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# A PROGRAM FOR EQUILIBRIUM NORMAL SHOCK AND STAGNATION POINT SOLUTIONS FOR ARBITRARY GAS MIXTURES

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# A PROGRAM FOR EQUILIBRIUM NORMAL SHOCK AND STAGNATION POINT SOLUTIONS FOR ARBITRARY GAS MIXTURES

By Linwood B. Callis and Jane T. Kemper
Langley Research Center

## SUMMARY

A computer program written in FORTRAN IV language is presented which yields solutions for flow parameters in arbitrary equilibrium gas mixtures in the following situations:

(1) Behind a normal shock

(2) Behind a reflected normal shock

(3) For in-flight stagnation conditions

(4) For shock-tube stagnation conditions

Program output parameters are pressure, density, enthalpy, entropy, compressibility, temperature, and mole fractions of the included chemical species, which may number up to thirty. For traveling normal and reflected shocks, the flow velocity and reflected shock velocity are also presented as output.

Equilibrium flow calculations are carried out by utilizing a free-energy minimization technique coupled with the steady-flow conservation equations and a modified Newton-Raphson iterative scheme. Chemistry up to second ionization is included.

Input required for the program is described and required physical constants for computations involving 27 species of the argon, nitrogen, oxygen, and carbon genre are tabulated. Cases may be run in sequence and any or all of the aforementioned flow configurations may be included in a single case.

Typical shock solutions are presented for argon free air and a model of the Mars atmosphere. Air solutions of the present work are compared with those from the Avco Corporation and Space Technology Laboratories.

## INTRODUCTION

Since the advent of hypervelocity vehicles and test facilities, it has been necessary in the solution for normal shock and stagnation point conditions to include the effects of the complex chemistry associated with high-speed phenomena. Since the equilibrium properties of high-temperature air are well known (refs. 1 to 6), there have been numerous solutions for normal shock parameters in air including stagnation point solutions (refs. 7 to 12). Methods of solution range from computer use of polynomial fits of equilibrium thermodynamic data to hand calculations (for example, refs. 9 and 11, respectively).

Recently, however, with the advancing sophistication and success of planetary probes it has become clear that programs should be available which are capable of determining thermochemical equilibrium shock parameters in a gas of arbitrary composition. One such program has been developed at the Avco Corporation and utilizes a free-energy minimization technique to get the equilibrium composition of the flow. This program, however, solves the shock problem inversely with values of temperature behind the shock being required in order to solve for the remaining shock properties, including shock speed.

It was believed by the present authors that another useful and somewhat more versatile means of solution might be realized by combining free-energy minimization techniques with a direct solution to the normal shock problem. The RAND method (ref. 13) of equilibrium gas analysis states the equilibrium problem simply and, when coupled with steepest descent techniques, is well suited to digital-computer use. This method is used in the present program with the conservation equations and a modified Newton-Raphson iterative scheme allowing direct solutions for thermodynamic and flow properties behind traveling and reflected normal shock waves and at in-flight and shock-tube stagnation points.

The program in FORTRAN IV language and the required program input are listed in full detail in appendixes A and B. Typical air solutions are presented and comparisons are made with solutions by Ziemer (ref. 11) and Laird and Heron (ref. 12). In addition, results from normal shock solutions in a Martian atmosphere (NASA model 2, ref. 14) are also presented and compared with air solutions.

The present program is used in conjunction with an IBM 7040-7094 direct coupled system. It is referred to as problem 886.5 and is available from the Analysis and Computation Division at Langley Research Center, Langley Station, Hampton, Virginia.

## SYMBOLS

| | |
|---|---|
| $f_T,f_p$ | perturbation parameters used in stagnation point solution |
| H | enthalpy |

| | |
|---|---|
| $\left[(H - T)_p\right]^{(r)}_{(n)}$ | parameter defined by equation (16) |
| $L$ | characteristic distance |
| $M$ | molecular weight |
| $M1$ | molecular weight of free-stream gas at 300° K |
| $N_e$ | number density of electrons |
| $p$ | pressure |
| $\mathcal{R}$ | universal gas constant |
| $R$ | universal gas constant divided by free-stream molecular weight |
| $S/R$ | nondimensional entropy |
| $S^{(k)}_{(n)}$ | parameter defined by equation (5) |
| $\left[(S - p)_H\right]^{(r)}$ | parameter defined by equation (23) |
| $\left[(S - T)_H\right]^{(r)}$ | parameter defined by equation (24) |
| $T$ | temperature |
| $U$ | characteristic velocity |
| $U_s,U_r$ | incident and reflected shock velocity, respectively |
| $u_2$ | flow velocity behind traveling incident shock in laboratory coordinates |
| $\bar{u}_2$ | velocity relative to shock |
| $X$ | mole fraction |
| $Z$ | compressibility factor, $M1/M$ |
| $\epsilon_{st}$ | convergence criterion in stagnation point solution |
| $\rho$ | density |
| $\rho_0$ | density of standard atmosphere |

| | |
|---|---|
| $\tau$ | characteristic time, L/U |
| $\omega_e, \omega_e x_e$ | spectroscopic constants |

Subscripts:

| | |
|---|---|
| 1 | conditions prior to shock |
| 2 | conditions behind incident shock in shock tube |
| 3 | conditions behind standing shock in shock tube |
| 5 | conditions behind reflected shock |
| st | shock-tube stagnation condition |
| sf | in-flight stagnation condition |
| (n) | refers to minor iteration in shock and stagnation routines |
| p | particular species (atom, molecule, ion, and electron) in free stream |
| i | particular species (atom, molecule, ion, and electron) behind shock |
| j | particular elemental component (atomic elements and electrons) |

Superscripts:

| | |
|---|---|
| (k) | refers to major iteration in shock routine |
| (r) | refers to major iteration in stagnation routine |

## EQUILIBRIUM PROPERTIES PROGRAM

The normal shock problem in thermochemical equilibrium is simply solved provided there is a straightforward means of handling the necessary equilibrium calculations. The RAND method is based on the principle that at given values of p and T, a constant-mass equilibrium mixture is so composed that its Gibbs free energy is at a minimum value. The composition yielding this minimum value is determined by making successive quadratic approximations to the free energy and using steepest descent techniques to converge upon a set of mole numbers yielding the minimum total free energy. This method permits the formulation of the equilibrium problem for an arbitrary gas in direct fashion and requires little or no chemical intuition.

The equilibrium program used in the present work, requiring p and T as thermodynamic input, is a version of the RAND method and is embodied in work done by Allison (ref. 15). This procedure utilizes the free energy minimization technique in conjunction with the partition function of quantum statistical mechanics to determine the free energies and enthalpies of the individual species and the equilibrium set of mole numbers (composition). This being done, thermodynamic parameters of interest are then determined. Assumptions involved in the use of partition functions in this analysis are as follows:

(1) For molecules the rigid rotor harmonic oscillator model is used, account being taken of the variation of vibrational and rotational constants due to different electronic configurations.

(2) Only electronic levels of energy (in the first five electron shells) lower than the ionization limit are considered for atoms and atomic ions.

Effects on thermodynamic properties of vibrational and rotational corrections to the model proposed are in general small (approximately 1 percent or less as shown in ref. 15) and for convenience are neglected in the present work. No further details, other than the equilibrium subroutine itself, are presented herein on this method of equilibirum gas analysis. Readers interested in these details should refer to references 13 and 15.

## ITERATIVE SOLUTION FOR CONSERVATION EQUATIONS

With an effective equilibrium program available, consideration must now be given as to which method of solution of the conservation equations is preferable, the direct or inverse method. The direct solution requires as input the preshock flow conditions, including the shock speed, and yields conditions behind the shock. The inverse solution requires the specification of T behind the shock with the subsequent solution for the remainder of the conditions both before and after the shock, including shock speed. The authors of the present report believe that the direct method has more general utility. Hence, the normal shock problem is approached in this fashion with the aid of a modified Newton-Raphson iterative technique (ref. 16) in conjunction with the shock-fixed conservation equations.

### Incident Shock

The conservation equations for the incident shock may be written as

$$\rho_2\bar{u}_2 = \rho_1 U_s \tag{1}$$

$$p_2 + \rho_2\bar{u}_2^2 = p_1 + \rho_1 U_s^2 \tag{2}$$

$$H_2 + \frac{1}{2}\,\bar{u}_2^2 = H_1 + \frac{1}{2}\,U_s^2 \tag{3}$$

where $\bar{u}_2$ is the velocity behind the shock relative to it and values of $T_1$, $p_1$, and $U_s$ are specified in the free stream.

For values of $T_1$ in excess of 800° K, values of $\rho_1$ and $H_1$, to be used in equations (1) to (3), are determined with the aid of the equilibrium program. Species included in this calculation are those which are to be considered behind the shock. This technique makes possible the generation of solutions with dissociating, high-temperature free streams. For lower values of $T_1$, the equilibrium program is again used to determine $\rho_1$ and $H_1$; however, the only species considered are those present at a temperature of 300° K.

Briefly, the iterative solution proceeds as follows:

(1) Assumed $\rho_2^{(k)}$ leads, with the aid of equations (1) to (3), to $p_2^{(k)}, H_2^{(k)}$. In principle, these two thermodynamic properties allow the evaluation of $\rho_2^{(k+1)}$ which is used once again in equations (1) to (3). This procedure, which shall be referred to as the major iteration, is repeated to convergence, solving the problem. In practice, however, the equilibrium program requires a $p,T$ input making necessary the Newton-Raphson iterative procedure (hereinafter called the minor iteration) in order to determine a value of $T_{(n)}^{(k)}$ compatible with the pressure and enthalpy solved for in the major iteration. With this temperature, or an approximation to it, $\rho_2^{(k+1)}$ is determined and the procedure repeated until the desired convergence between $\rho_2^{(k)}$ and $\rho_2^{(k+1)}$ is achieved. The superscript (k) refers to the kth major iteration and the subscript (n) is associated with the minor iterations.

(2) The recursive equations used in the minor iteration are

$$T_{(n+1)}^{(k)} = T_{(n)}^{(k)} + \frac{H_2^{(k)} - H_{(n)}^{(k)}}{S_{(n)}^{(k)}} \tag{4}$$

where

$$S_{(n)}^{(k)} = \frac{H_{(n)}^{(k)} - H_{(n-1)}^{(k)}}{T_{(n)}^{(k)} - T_{(n-1)}^{(k)}} \tag{5}$$

To begin this iteration, it is necessary to input an estimated temperature $T_{(0)}^{(1)}$ and an initial temperature increment $\Delta T$. The sum of these is given as

$$T_{(1)}^{(1)} = T_{(0)}^{(1)} + \Delta T \tag{6}$$

which is used in the first approximation. Values of the enthalpy $H_{(n)}^{(k)}$ in equations (4) and (5) are determined from the equilibrium program with $p_2^{(k)}$ and $T_{(n)}^{(k)}$ as input and are computed with each successive value of $T_{(n)}^{(k)}$ as are values of the parameter $S_{(n)}^{(k)}$ given by equation (5).

(3) The program is arranged so that for $k = 1$ there are three minor iterations beginning with the computations of an improved value of $T_{(1)}^{(1)}$. For each successive value of $k$ only one minor iteration is made, use being made of the following relations:

$$S_{(1)}^{(k+1)} = S_{\text{last}}^{(k)} \qquad (k \geqq 1) \tag{7}$$

$$T_{(1)}^{(k+1)} = T_{\text{last}}^{(k)} \qquad (k \geqq 1) \tag{8}$$

where $S_{\text{last}}^{(k)}$ and $T_{\text{last}}^{(k)}$ are simply the last values of these quantities computed during the kth major iteration. When the final value of $T_{(n)}^{(k)}$ has been computed, $T_{(n)}^{(k)}$ and $p_2^{(k)}$ are used in the equilibrium program to evaluate $\rho_2^{(k+1)}$ which is compared with $\rho_2^{(k)}$ to determine whether the specified convergence criterion has been satisfied. If the criterion has not been satisfied, $\rho_2^{(k+1)}$ is used in equations (1) to (3) to obtain $p_2^{(k+1)}$ and $H_2^{(k+1)}$. The cycle is continued until convergence requirements are satisfied.

Solutions to the problem are presented with reference to a laboratory coordinate system.

One comment by way of explanation should be made about the scheme of minor iterations. The minor iterations are not continued to the point where a value of $T_{(n)}^{(k)}$ completely compatible with $p_2^{(k)}$ and $H_2^{(k)}$ is realized. These iterations are truncated early in favor of obtaining swiftly a value of $\rho_2^{(k+1)}$. Experience has justified this procedure since it has been observed that the major correction to the estimated temperature occurs during the first three minor iterations. Subsequent iterations are refinements, eliminated in favor of determining a new approximation to the density and continuing the major iteration. This procedure has no bearing on the final accuracy achieved, inasmuch as this accuracy is dependent on the convergence criterion specified for successive values of $\rho^{(k)}$.

## Reflected Shock

The conservation equations for the reflected shock may be written in shock-fixed coordinates as

$$\rho_2(u_2 + U_r) = \rho_5 U_r \tag{9}$$

$$p_2 + \rho_2(u_2 + U_r)^2 = p_5 + \rho_5 {U_r}^2 \tag{10}$$

$$H_2 + \frac{1}{2}(u_2 + U_r)^2 = H_5 + \frac{1}{2} {U_r}^2 \tag{11}$$

where all velocities are relative to a laboratory reference system and conditions behind the incident shock will have been determined from the incident shock program.

For the sake of brevity, it should suffice to say that the major and minor iterative schemes, including the initial input, are identical in every detail to those for the incident shock. Only the form of the conservation equations to be used in the major iteration differs in the two situations. For this reason, no further comment on the reflected shock solution is made except to indicate that results are presented in a laboratory reference frame. Such reference results in zero flow velocity behind the reflected wave, as expected.

## In-Flight Stagnation Conditions

In-flight stagnation conditions are determined by solving the incident shock problem and locating a thermodynamic state point so that the conditions

$$H_{sf} = H_1 + \frac{1}{2} U_s^2 \tag{12}$$

$$(S/R)_{sf} = (S/R)_2 \tag{13}$$

are satisfied. With the present equilibrium program, equations (12) and (13) are achieved with the greatest facility by means of a two-dimensional Newton-Raphson iterative process. This procedure, for purposes of brevity and clarity, is presented as a series of comments or computational procedures, as follows:

(1) The series of iterations is initiated with the following pressures and temperatures:

$$\left.\begin{aligned} p^{(1)} &= p_2 \\ p^{(2)} &= p_2\left(1 + f_p\right) \\ T^{(1)}_{(0)} &= T_2 \\ T^{(1)}_{(1)} &= T_2\left(1 + f_T\right) \end{aligned}\right\} \tag{14}$$

where $f_p$ and $f_T$ are small perturbation parameters required as input. Superscripts and subscripts within parentheses refer respectively to the number of approximations to $p_{sf}$ and the number of iterations on temperature at constant $p^{(r)}$.

(2) By utilizing equations (14) when applicable and

$$T^{(r)}_{(n+1)} = T^{(r)}_{(n)} + \frac{H_{sf} - H^{(r)}_{(n)}}{\left[(H - T)_p\right]^{(r)}_{(n)}} \qquad ((n) \geqq 1) \tag{15}$$

where

$$\left[(H - T)_p\right]^{(r)}_{(n)} = \frac{H^{(r)}_{(n)} - H^{(r)}_{(n-1)}}{T^{(r)}_{(n)} - T^{(r)}_{(n-1)}} \tag{16}$$

$$\left[(H - T)_p\right]_{(1)}^{(r)} = \left[(H - T)_p\right]_{last}^{(r-1)} \qquad ((r) > 1) \tag{17}$$

$$T_{(1)}^{(2)} = T_{last}^{(1)} \tag{18}$$

successive values of temperature are determined until a value of $T_{last}^{(r)}$ is reached so that

$$\left|\frac{H_{last}^{(r)} - H_{sf}}{H_{sf}}\right| \leqq \epsilon_{st} \tag{19}$$

where $\epsilon_{st}$ is a predetermined small quantity. Entropy convergence according to

$$\left|\frac{(S/R)_{last}^{(r)} - (S/R)_{sf}}{(S/R)_{sf}}\right| \leqq \epsilon_{st} \tag{20}$$

is also checked at this point in the solution. If condition (20) is met, the stagnation-point conditions are determined. If convergence is not achieved, use the following procedure.

(3) Determine new values of $p$ and $T$ from

$$p^{(r+1)} = p^{(r)} + \frac{(S/R)_{sf} - (S/R)_{last}^{(r)}}{\left[(S - p)_H\right]^{(r)}} \qquad (r \geqq 2) \tag{21}$$

$$T_{(1)}^{(r+1)} = T_{last}^{(r)} + \frac{(S/R)_{sf} - (S/R)_{last}^{(r)}}{\left[(S - T)_H\right]^{(r)}} \qquad (r \geqq 2) \tag{22}$$

where

$$\left[(S - p)_H\right]^{(r)} = \frac{(S/R)_{last}^{(r)} - (S/R)_{last}^{(r-1)}}{p^{(r)} - p^{(r-1)}} \qquad (r \geqq 2) \tag{23}$$

$$\left[(S - T)_H\right]^{(r)} = \frac{(S/R)_{last}^{(r)} - (S/R)_{last}^{(r-1)}}{T_{last}^{(r)} - T_{last}^{(r-1)}} \qquad (r \geqq 2) \tag{24}$$

(4) With the new values of pressure and temperature reenter step (2) and continue the cycle until both enthalpy and entropy meet the convergence test (eqs. (19) and (20)). This procedure, then, satisfies requirements (12) and (13) to the desired degree of accuracy and the problem is complete.

All values of enthalpy and entropy are determined from the equilibrium program.

## Shock-Tube Stagnation Conditions

The solution for shock-tube stagnation conditions requires two incident shock solutions followed by a Newton-Raphson iteration in two dimensions. The incident shock solution, described previously, yields solutions for conditions which serve as input required to determine conditions behind the standing shock. This solution, used once again, determines conditions behind the standing shock which, when coupled with the two-dimensional iteration described in the previous section, are then used to determine a thermodynamic state point so that

$$H_{st} = H_2 + \frac{1}{2} u_2^2 \tag{25}$$

$$(S/R)_{st} = (S/R)_3 \tag{26}$$

with the required degree of convergence specified. The solution reached in this manner is that of the shock-tube stagnation point.

The program, briefly described in the preceding sections, is listed in FORTRAN IV language in appendix A with a description and explanation of the input required given in appendix B. Appendix C presents a compilation of physical constants, most of which may be found itemized with regard to their source in reference 15 and references 17 to 20. These constants are required by the program for use with the 27 chemical species indicated.

## LIMITATIONS

Limitations on the present normal shock program are those restrictions placed on the equilibrium properties program. It is recommended in reference 15 that the present version of the RAND method of computing the equilibrium compositions be restricted to pressures below $10^2$ atmospheres; thus, real-gas effects manifested at higher pressures are avoided. Such effects, for air, are taken into account in the work of Lewis and Burgess (ref. 7), which allows consideration of pressures several orders of magnitude higher than the upper limit suggested for the present work.

The present equilibrium program is valid down to pressures at which the assumptions inherent in the theory of statistical thermodynamics begin to fail. However, when a flow process is considered, pressures must be such that the response times of thermodynamic parameters to a change in condition must be much smaller than the characteristic time $\tau$ associated with the problem. Such decisions are left to the discretion of the individual investigator.

Temperatures considered must be such that only negligible contributions are realized from coulomb interactions and from electronic energy levels past the fifth electron shell, both these considerations being unaccounted for in the equilibrium program. The latter consideration proves to be no problem for temperatures below 15 000° K; however, this temperature cannot be said to be a lower universal limit for the neglect of coulomb effects. These effects depend, in addition to temperature, on the pressure and the gas mixture considered. The problem therefore becomes one for the individual investigator depending on the particular circumstances at hand.

## COMPARISON OF SOLUTIONS

As an indication of the versatility and validity of the present computer program, comparisons are made with the work of Laird and Heron (ref. 12) and Ziemer (ref. 11).

In figure 1, the flow configurations used in this study are illustrated. In figures 2 to 5 normal shock properties in argon free and carbon free air as determined from the present program are compared with those of Laird and Heron (ref. 12). The initial mixture considered, at $p_1 = 76$ and $10^{-3}$ cm Hg and $T_1 = 300^\circ$ K, was composed of 21.153 percent $O_2$ and 78.847 percent $N_2$ by volume. Species considered were $NO^+$, NO, $O_2^+$, $O_2$, $N_2^+$, $N_2$, $O^-$, $O^+$, $O^{++}$, O, $N^{++}$, $N^+$, N, $e^-$, $N_2O$ excluding $N^-$ which was included in reference 12. Figures 2 to 5 indicate excellent agreement, small discrepancies being noted in $T$ and $\rho$ for $T > 18\ 000^\circ$ K. These discrepancies, however, remain below 3 percent. Although only data for the incident shock and the shock-tube stagnation conditions are shown, standing shock and reflected shock data compare equally well.

In figures 6 and 7, comparisons are shown between the data of Ziemer (ref. 11) and data from the present program in which the previously described air model was used. The data of Ziemer was generated by using a graphical representation of the equilibrium air analysis of reference 1. The comparisons, which are made for incident and reflected shock data, at two initial pressures and $T_1 = 273.2^\circ$ K, show considerably larger discrepancies in $T$ and $\rho$ than the Avco data, sometimes reaching 12 percent. These discrepancies, previously pointed out by Hoshizaki (ref. 21), are attributed to errors in Ziemer's data which, according to Ziemer, have an estimated accuracy of 1 to 10 percent.

No comparisons, for identical flow conditions, have been made of solutions discussed in the present section. It was believed that the interpolation required between references 11 and 12 would only compound existing discrepancies.

In figure 8, a comparison is made between the incident shock properties of the present air model and a Martian atmosphere (NASA model 2, ref. 14). The Mars atmosphere consists of an initial mixture of 10.8 percent $CO_2$ and 89.2 percent $N_2$ by volume. Species considered in the Martian atmosphere were N, $N^+$, $N^{++}$, O, $O^+$, $O^{++}$, $O^-$, C, $C^+$, $C^{++}$, $C^-$, $N_2$, $N_2^+$, $O_2$, $O_2^+$, NO, $NO^+$, CO, $CO^+$, CN, $CO_2$, $e^-$. Initial conditions of both mixtures were taken to be $p_1 = 10^{-1}$ atmosphere and $T_1 = 273.2^\circ$ K.

Finally, comparisons made in reference 15 of equilibrium air properties as generated by the present equilibrium program with the more rigorous data of Gilmore (ref. 1) and Browne (ref. 22) generally agree within 1 percent for $1000^\circ \text{ K} \leqq T \leqq 25\,000^\circ \text{ K}$ and $10^{-6} \leqq \rho/\rho_0 = 10$.

## CONCLUDING REMARKS

The present program has proved capable of accurately determining both flow and thermodynamic parameters behind incident and reflected shock waves and at stagnation points for both in-flight and shock-tube thermochemical equilibrium flow. Capable of handling arbitrary free-stream mixtures and gas chemistry (up to second ionization), the solution provides a convenient means of solving directly for the flow parameters if the free-stream pressure, temperature, velocity, and composition are given.

Langley Research Center,
National Aeronautics and Space Administration,
Langley Station, Hampton, Va., October 6, 1965.

## APPENDIX A

## PROGRAM FOR CALCULATION OF NORMAL SHOCK AND STAGNATION-POINT CONDITIONS

The program for calculating flow parameters in thermochemical equilibrium for normal shock and stagnation-point conditions in arbitrary gas mixtures was written in FORTRAN IV language for the IBM 7094 electronic data processing system. This program including subroutines and comments is reproduced in the following pages.

# APPENDIX A

```
$IBFTC P8865
C
C             P-886.5
C          NORMAL SHOCK PROGRAM
C          PROGRAMMED FOR THE IBM 7094
C       YIELDING SOLUTIONS FOR FLOW PARAMETERS IN ARBITRARY GAS
C      MIXTURES IN THE FOLLOWING SITUATIONS-
C               1. BEHIND NORMAL SHOCK
C               2. BEHIND A REFLECTED NORMAL SHOCK
C               3. FOR IN FLIGHT STAGNATION CONDITIONS
C               4. FOR SHOCK TUBE STAGNATIONS CONDITIONS
C
      DIMENSION OMEG(5,30,30),F(30),CAPM(30),A(10,30),L(30),
     1G(30,30),SMALE(30,30),X(30),CAPLAM(30,30),DHFO(30),YSTO(30)
C
      DIMENSION CP(5),BETA(5),AM(5),CODE(30),SHBL(8),REBL(8),STBL(8),
     1STSBL(8),NBTA(5)
      DIMENSION TEMP(5)
      DIMENSION YSAVE(30)
C
C     EQUILIBRIUM INPUT
C
      COMMON OMEG,F,CAPM,A
      COMMON G,SMALE
      COMMON CONH,CONK,CONR,CONPRF,CONNO,N,M,L,NIT
      COMMON EPS1,EPS2,CAPLAM
      COMMON DHFO,AMC,IC1,YSTO
C
C      SHOCK PROGRAM INPUT
C
      COMMON P10,T10,US,RHO2,EPS5,NB,CP,BETA,AM,TP,DELT,IT,NBTA
C
C     REFL INPUT
C
      COMMON TR,RHOR
C
C
C     STAG INPUT
C
      COMMON FP,FT,ES
C
C     ST-STAG INPUT
C
      COMMON TSTAG,RHOS
C
      COMMON SHBL,STBL,STSBL,REBL,SOR,X
C
      WRITE (6,200)
  200 FORMAT(1H1,20H EQUILIBRIUM PROGRAM//27H JANE KEMPER FOR LIN CALLIS
```

```
     1//30H J. O. RGH-125 PROB. NO. 886.5///)
C
C     THE FIRST N+1 DATA CARDS CONTAIN INFORMATION (IN COLUMNS 1-6)
C     IDENTIFYING EACH OF THE N SPECIES.  THE FIRST CARD IS N (COL. 1-3)
C
      READ(5,205)NCODE
  205 FORMAT(I3)
      READ(5,206)(CODE(I),I=1,NCODE)
  206 FORMAT(1A6)
C
C     LOAD INPUT   ALL DATA (AFTER FIRST N+1 CARDS) IS ON DEC CARDS
C        LAST CARD IS FOLLOWED BY A TRA 2,4 CARD
C
    1 CALL LOAD(NERR)
C
C     NERR  CONTAINS LOADING CODE
C                    =1 PROPER LOADING, COMPUTE
C                    =2 ERROR,  CARD IN ERROR WILL BE PRINTED, EXIT
C                    =3 END OF FILE,  EXIT
C
      IF(NERR-2)4,3,2
    2 CONTINUE
    3 CALL EXIT
    4 N=N
      READ (5,205)ITEST
C
C     ITEST  CONTAINS CODE FOR OPTIONS (PUNCHED IN COL. 3 ON CARD
C          FOLLOWING TRA CARD AFTER LAST DATA CARD)
C     POSSIBLE OPTIONS
C        0      INCIDENT SHOCK ONLY
C        1      INC. AND REFLECTED SHOCKS
C        2      INC. AND FREE STREAM STAGNATION
C        3      INC., FREESTREAM STAG., AND REFL.
C        4      INC. AND SHOCK TUBE STAGNATION
C        5      INC., SHOCK TUBE STAG. AND REFL.
C        6      INC., SHOCK TUBE AND FREESTREAM STAGNATION
C        7      INC., SHOCK TUBE STAG., FREESTREAM STAG. AND REFL.
C
      M=M
      CALL SLITE(0)
      RHO10=P10/(T10/300.)*.040619*AMC
      DO 5 I=1,NB
      I1=NBTA(I)
    5 TEMP(I)=CODE(I1)
      WRITE(6,4000)RHO10,P10,US,T10,(TEMP(I),I=1,NB)
 4000 FORMAT(1H125H INPUT FOR INCIDENT SHOCK//8H RHO-1 =E15.8,2X,
     15HP-1 =E15.8,2X,3HUS=E15.8,2X,5HT-1 =E15.8//5H BETA//(5(9X,1A6,2X)
     2))
      WRITE(6,4001)(BETA(I),I=1,NB)
 4001 FORMAT(5E17.8)
      WRITE(6,4002)RHO2
```

```
 4002 FORMAT(//13H ASSUMED RHO=E15.8)
C      CONVERSION
       P10=P10*1.01325E6
       RHO10=RHO10*1.E-3
       RHO2=RHO2*1.E-3
       US=US*30.48
       DO 3004 I=1,N
 3004 YSAVE(I)=YSTO(I)
C
C      IF T10 LESS THAN 800 DEGREES KELVIN, COMPUTE ENTHALPY (H10)
C           FROM FREESTREAM COMPOSITION (USING SUBROUTINE ECOM)
C      IF T10 GREATER THAN 800. DEGREES, SOLVE FOR ENTHALPY
C           ITERATIVELY USING SUBROUTINE ECOM
C
       IF(T10 -800.)3003,3003,3006
 3003 DO 3005 I=1,N
 3005 YSTO(I)=0.
C
C      SENSE LIGHT 4 USED TO SIGNAL SUBROUTINE ECOM
C
       CALL SLITE(4)
       DO 3035 I=1,NB
       J=NBTA(I)
 3035 YSTO(J)=BETA(I)/AMC
 3006 C=2.99793E10
       CALL ECOM(T10,P10,OOZ,HOZRT,H10,RHO10)
       DO 3007 I=1,N
 3007 YSTO(I)=YSAVE(I)
C
C      STORE INITIAL P,T,RHO,AND U IN SHBL(1-4)
C
       SHBL(1)=P10
       SHBL(2)=T10
       SHBL(3)=RHO10
       SHBL(4)=US
       CALL SHOCK(TP,OOZ,HOZRT,H2,SHBL,H10,NN)
C
C      UPON RETURN SHBL(5-8) CONTAINS P2,T2,RHO2,AND UF
C
       PPRINT=SHBL(5)/CONPRF
C
       UPRINT=SHBL(8)/30.48
C
       WRITE(6,4003)UPRINT,NN
 4003 FORMAT(////7H OUTPUT//5H U2 =E15.8,20X,25HNO. OF MAJOR ITERATIONS
     1=I3)
C
 2050 WRITE(6,202)PPRINT,SHBL(7),OOZ,HOZRT,SOR,SHBL(6),AMC
  202 FORMAT(//9X,1HP,13X,3HRHO,14X,3H1/Z,14X,5HH/ZRT,12X,3HS/R,
     114X,1HT,16X,2HM1//(7E17.8))
       WRITE(6,221)
```

```
  221 FORMAT(//23H FINAL X FROM ITERATION,4X,7HSPECIES//)
      WRITE(6,220)(X(I),CODE(I),I=1,N)
  220 FORMAT(E17.8,10X,1A6)
C
C     STORE S/R FOR STAG AND STSTAG SUBROUTINES
C
      STBL(3)=SOR
C
C     TEST FOR ADDITIONAL OPTIONS
C
    9 IF(ITEST)1,1,10
   10 IC=1
C
  105 IF(ITEST-IC)1,11,12
   11 GO TO (15,20,15,25,25,25,25),IC
C
   12 IC=IC+1
      GO TO 105
C
   15 WRITE(6,4004)RHOR
 4004 FORMAT(1H1,16H REFLECTED SHOCK//17H     ASSUMED RHO =E15.8)
      RHOR=RHOR*1.E-3
C
C     STORE P2,T2,RHO2, AND UF IN REBL(1-4)
C
      REBL(1)=SHBL(5)
      REBL(2)=H2
      REBL(3)=SHBL(7)*1.E-3
      REBL(4)=SHBL(8)
      CALL REFL(TR,OOZ,HOZRT,NN)
C
C     UPON RETURN REBL(5-8) CONTAINS PR,TR,RHOR,AND UR
C
      UPRINT=REBL(8)/30.48
      PPRIN=REBL(5)/CONPRF
      WRITE(6,5003)UPRINT,NN
 5003 FORMAT(///7H OUTPUT//5H U-R=E15.8,20X,25HNO. OF MAJOR ITERATIONS =
     1I3)
C
      WRITE(6,202)PPRIN,REBL(7),OOZ,HOZRT,SOR,REBL(6),AMC
      WRITE(6,221)
      WRITE(6,220)(X(I),CODE(I),I=1,N)
      ITEST=ITEST-1
      GO TO 10
   20 HS=H10+(SHBL(4)**2)/2.
      WRITE(6,5004)HS,STBL(3)
 5004 FORMAT(1H1,76H  IN FLIGHT STAGNATION POINT DATA IS COMPUTED FROM T
     1HE INCIDENT SHOCK OUTPUT//22H STAGNATION ENTHALPY =E15.8,5X,
     220HSTAGNATION ENTROPY =E15.8/////)
C
C     STORE P2, AND T2 IN STBL(1-2)  ,     H2 IN STBL(4)
```

```
C
      STBL(1)=SHBL(5)
      STBL(2)=SHBL(6)
      STBL(4)=H2
      CALL STAG(HS,OOZ,HOZRT,RHO,STBL,NN)
C
C     UPON RETURN STBL(5-8) CONTAINS P-ST, T-ST, S/R-ST, AND H-ST
C
      PPRIN=STBL(5)/CONPRF
      WRITE(6,5005)PPRIN,STBL(6),NN,OOZ,HOZRT,RHO,STBL(7),STBL(8)
 5005 FORMAT(///7H OUTPUT//15H     PRESSURE =E15.8,18H      TEMPERATURE =
     1E15.8,22X,25HNO. OF MAJOR ITERATIONS =I3//6H 1/Z =E15.8,5X,
     X7HH/ZRT =E15.
     28,5X,5HRHO =E15.8,5X,5HS/R =E15.8,5X,3HH =E15.8)
      WRITE(6,221)
      WRITE(6,220)(X(I),CODE(I),I=1,N)
      ITEST=ITEST-2
      GO TO 10
C
C     TO COMPUTE THE SHOCK TUBE STAGNATION POINT PROPERTIES, SUBROUTINE
C     SHOCK IS USED FOR THE STANDING SHOCK DATA.  THEN SUBROUTINE
C     STAG COMPUTES THE STAGNATION POINT DATA.
C
C     STORE P2,T2,RHO2, AND UF IN STSBL(1-4)
C
   25 STSBL(1)=SHBL(5)
      STSBL(2)=SHBL(6)
      STSBL(3)=SHBL(7)*1.E-3
      RHO2=RHOS*1.E-3
      STSBL(4)=SHBL(8)
      CALL SHOCK(TSTAG,OOZ,HOZRT,HST,STSBL,H2,NN)
      HS=H2+(SHBL(8)**2)/2.
      PPRINT=STSBL(5)/CONPRF
      UPRINT=STSBL(8)/30.48
      WRITE(6,5006)
 5006 FORMAT(1H1,84H SHOCK TUBE STAGNATION POINT DATA IS COMPUTED FROM T
     1HE FOLLOWING STANDING SHOCK DATA)
      WRITE(6,202)PPRINT,STSBL(7),OOZ,HOZRT,SOR,STSBL(6),AMC
      WRITE(6,5007)HS
 5007 FORMAT(//39H SHOCK TUBE STAGNATION POINT ENTHALPY =E17.8/)
C
C     STORE P,T, AND H VALUES FROM SECOND ENTRY INTO INCIDENT SHOCK
C        SUBROUTINE IN STSBL(1-2,4)
C
C     STORE S/R-2 IN STSBL(3)
C
      STSBL(1)=STSBL(5)
      STSBL(2)=STSBL(6)
      STSBL(3)=SOR
      STSBL(4)=HST
      CALL STAG(HS,OOZ,HOZRT,RHO,STSBL,NN)
```

```
C
C      UPON RETURN STSBL(5-8) CONTAINS P-STS, T-STS, S/R-STS, AND H-STS
C
       PPRINT=STSBL(5)/CONPRF
       WRITE(6,5005)PPRINT,STSBL(6),NN,OOZ,HOZRT,RHO,STSBL(7),STSBL(8)
       WRITE(6,221)
       WRITE(6,220)(X(I),CODE(I),I=1,N)
       ITEST=ITEST-4
       GO TO 10
       END
```

```
$IBFTC SHOCK
       SUBROUTINE SHOCK(TGUESS,OOZ,HOZRT,H2,BLOCK,H10,NCOUNT)
C
C      THIS SUBROUTINE USES A ONE-DIMENSIONAL NEWTON-RAPHSON ITERATION
C      SCHEME TO FIND TEMPERATURE AND PRESSURE AT EQUILIBRIUM BEHIND
C      INCIDENT SHOCK.  IT WILL CALL SUBROUTINE ECOM TO COMPUTE THE
C      EQUILIBRIUM PROPERTIES.
C
C      H10 IS INITIAL ENTHALPY
C      TGUESS IS TEMPERATURE ESTIMATE
C      BLOCK(1-4) CONTAINS INITIAL P,T,DENSITY AND VELOCITY
C           FINAL VALUES OF P,T,DENSTIY AND VELOCITY STORED IN BLOCK(5-8)
C      ENTHALPY STORED AT H2
C      NCOUNT IS AN ITERATION COUNT
C      1/Z, H/ZRT STORED IN OOZ AND HOZRT
C
C
       DIMENSION OMEG(5,30,30),F(30),CAPM(30),A(10,30),L(30),
      1G(30,30),SMALE(30,30),X(30),CAPLAM(30,30),DHFO(30),YSTO(30)
       DIMENSION CP(5),BETA(5),AM(5),SHBL(8),REBL(8),STBL(8),STSBL(8),
      1NBTA(5)
       DIMENSION T(2),H(2),BLOCK(8)
       COMMON OMEG,F,CAPM,A
       COMMON G,SMALE
       COMMON CONH,CONK,CONR,CONPRF,CONNO,N,M,L,NIT
       COMMON EPS1,EPS2,CAPLAM
       COMMON DHFO,AMC,IC1,YSTO
       COMMON P10,T10,US,RHO2,EPS5,NB,CP,BETA,AM,TP,DELT,IT,NBTA
       COMMON TR,RHOR
```

APPENDIX A

```
      COMMON FP,FT,ES
      COMMON TSTAG,RHOS
C
      COMMON SHBL,STBL,STSBL,REBL,SOR,X
C
C     LET RHO2 = FIRST RHO
C
      VEL1(AA)=C*D/AA
      PRES1(AA,BB)=B+C*D**2-AA*BB**2
      ENTH1(AA)=H10+(D**2)/2.-(AA**2)/2.
      NCOUNT=1
      B=BLOCK(1)
      C=BLOCK(3)
.     D=BLOCK(4)
      U2=VEL1(RHO2)
      P2=PRES1(RHO2,U2)
      H2=ENTH1(U2)
C
C     COMPUTE FIRST POINT
C
      ITT=IT
    7 T(1)=TGUESS
      CALL ECOM(T(1),P2,OOZ,HOZRT,H(1),RHO)
C
C     COMPUTE SECOND POINT
C
      T(2)=T(1)+DELT
      CALL ECOM(T(2),P2,OOZ,HOZRT,H(2),RHO)
      S=(H(2)-H(1))/(T(2)-T(1))
      T(1)=T(2)
C
C     TEMPERATURE FROM FIRST ITERATION
C
      T(2)=T(2)+(H2-H(2))/S
      H(1)=H(2)
      IF(T(2))25,25,8
    8 CALL ECOM(T(2),P2,OOZ,HOZRT,H(2),RHO)
C
C     S IS SLOPE     (H2-H1)/(T2-T1)
C
   85 S=(H(2)-H(1))/(T(2)-T(1))
C     T3
      T(1)=T(2)
C
C     TEMPERATURE FROM SECOND ITERATION
C
      T(2)=T(2)+(H2-H(2))/S
      H(1)=H(2)
      IF(T(2))25,25,9
    9 CALL ECOM(T(2),P2,OOZ,HOZRT,H(2),RHO)
C
```

```
C     IF ITT IS GREATER THAN 2, ITERATE AGAIN ON TEMPERATURE WITH
C          FIRST PRESSURE
C
      IF(ITT-2)10,10,11
   10 SLAST=(H(2)-H(1))/(T(2)-T(1))
      TLAST=T(2)
      GO TO 12
C
   11 ITT=ITT-1
      GO TO 85
C
C
C     TEST RHO FOR CONVERGENCE
C
   12 IF(ABS((RHO-RHO2)/RHO2)-EPS5)20,20,13
C
C     NON-CONVERGENCE-
C
C     COMPUTE NEW PRESSURE AND CONTINUE ITERATION ON TEMPERATURE AND
C          PRESSURE UNTIL RHO CONVERGES
C
   13 RHO2=RHO
      U2=VEL1(RHO2)
      P2=PRES1(RHO2,U2)
      H2=ENTH1(U2)
      NCOUNT=NCOUNT+1
      T(1)=TLAST
   14 CALL ECOM(T(1),P2,OOZ,HOZRT,H(1),RHO)
  145 S=SLAST
   15 T(2)=T(1)+(H2-H(1))/S
      CALL ECOM(T(2),P2,OOZ,HOZRT,H(2),RHO)
      SLAST=(H(2)-H(1))/(T(2)-T(1))
      TLAST=T(2)
      GO TO 12
C
C     CONVERGENCE -  STORE OUTPUT
C
   20 U2=VEL1(RHO)
      UF=US-U2
      RHO=RHO*1.E3
      BLOCK(5)=P2
      BLOCK(6)=TLAST
      BLOCK(7)=RHO
      BLOCK(8)=UF
      RETURN
C
C     TEMPERATURE ESTIMATE TOO HIGH      -  ADJUST
C
   25 TGUESS=(TGUESS-T10)/2.
      GO TO 7
      END
```

APPENDIX A

```
$IBFTC REFL
      SUBROUTINE REFL(TGUESS,OOZ,HOZRT,NCOUNT)
C
C     THIS SUBROUTINE USES A ONE-DIMENSIONAL NEWTON-RAPHSON ITERATION
C     SCHEME TO FIND TEMPERATURE AND PRESSURE AT EQUILIBRIUM BEHIND
C     REFLECTED SHOCK.  IT WILL CALL SUBROUTINE ECOM TO COMPUTE THE
C     EQUILIBRIUM PROPERTIES.
C
      DIMENSION OMEG(5,30,30),F(30),CAPM(30),A(10,30),L(30),
     1G(30,30),SMALE(30,30),X(30),CAPLAM(30,30),DHFO(30),YSTO(30)
      DIMENSION CP(5),BETA(5),AM(5),SHBL(8),REBL(8),STBL(8),STSBL(8),
     1NBTA(5)
      DIMENSION T(2),H(2)
C
      COMMON OMEG,F,CAPM,A
      COMMON G,SMALE
      COMMON CONH,CONK,CONR,CONPRF,CONNO,N,M,L,NIT
      COMMON EPS1,EPS2,CAPLAM
      COMMON DHFO,AMC,IC1,YSTO
      COMMON P10,T10,US,RHO2,EPS5,NB,CP,BETA,AM,TP,DELT,IT,NBTA
      COMMON TR,RHOR
      COMMON FP,FT,ES
      COMMON TSTAG,RHOS
C
      COMMON SHBL,STBL,STSBL,REBL,SOR,X
C
C     LET RHOR = FIRST RHO
C
      VEL(AA)=C*D/(AA-C)
      PRES(AA,BB)=B+C*(AA+D)**2-BB*AA**2
      ENTH(AA)=E+.5*(D+AA)**2-.5*AA**2
      NCOUNT=1
      B=REBL(1)
      C=REBL(3)
      D=REBL(4)
      E=REBL(2)
      UR=VEL(RHOR)
      PR=PRES(UR,RHOR)
      HR=ENTH(UR)
C
C     COMPUTE FIRST POINT
C
```

```
    7 T(1)=TGUESS
      CALL ECOM(T(1),PR,OOZ,HOZRT,H(1),RHO)
C
C     COMPUTE SECOND POINT
C
      T(2)=T(1)+DELT
      CALL ECOM(T(2),PR,OOZ,HOZRT,H(2),RHO)
C
C     S IS SLOPE    (H2-H1)/(T2-T1)
C
      S=(H(2)-H(1))/(T(2)-T(1))
      T(1)=T(2)
C
C     TEMPERATURE FROM FIRST ITERATION
C
      T(2)=T(2)+(HR-H(2))/S
      H(1)=H(2)
      IF(T(2))25,25,8
    8 CALL ECOM(T(2),PR,OOZ,HOZRT,H(2),RHO)
   85 S=(H(2)-H(1))/(T(2)-T(1))
      T(1)=T(2)
C
C     TEMPERATURE FROM SECOND ITERATION
C
      T(2)=T(2)+(HR-H(2))/S
      H(1)=H(2)
      IF(T(2))25,25,9
    9 CALL ECOM(T(2),PR,OOZ,HOZRT,H(2),RHO)
C
C     IF ITT IS GREATER THAN 2, ITERATE AGAIN ON TEMPERATURE WITH
C          FIRST PRESSURE
C
      IF(IT-2)10,10,11
   10 SLAST=(H(2)-H(1))/(T(2)-T(1))
      TLAST=T(2)
      GO TO 12
C
   11 ITT=ITT-1
      GO TO 85
C
C     TEST RHO FOR CONVERGENCE
C
   12 IF(ABS((RHO-RHOR)/RHOR)-EPS5)20,20,13
C
C
C     NON-CONVERGENCE-
C     COMPUTE NEW PRESSURE AND CONTINUE ITERATION ON TEMPERATURE AND
C          PRESSURE UNTIL RHO CONVERGES
C
   13 RHOR=RHO
      UR=VEL(RHOR)
```

```
      PR=PRES(UR,RHOR)
      HR=ENTH(UR)
      NCOUNT=NCOUNT+1
      T(1)=TLAST
      CALL ECOM(T(1),PR,OOZ,HOZRT,H(1),RHO)
      S=SLAST
      T(2)=T(2)+(HR-H(2))/S
      CALL ECOM(T(2),PR,OOZ,HOZRT,H(2),RHO)
      SLAST=(H(2)-H(1))/(T(2)-T(1))
      TLAST=T(2)
      GO TO 12
C
C
C     CONVERGENCE -  STORE OUTPUT
C
   20 UR=VEL(RHO)
      RHO=RHO*1.E3
      REBL(5)=PR
      REBL(6)=TLAST
      REBL(7)=RHO
      REBL(8)=UR
      RETURN
C
C     TEMPERATURE ESTIMATE TOO HIGH       -    ADJUST
C
   25 TGUESS=(TGUESS-T10)/2.
      GO TO 7
      END
```

```
$IBFTC STAG
      SUBROUTINE STAG(HS,OOZ,HOZRT,RHO,BLOCK,NN)
C
C     THIS SUBROUTINE USES A TWO DIMENSION NEWTON-RAPHSON ITERATION
C     SCHEME TO COMPUTE FREESTREAM OR SHOCK TUBE STAGNATION POINT
C     PRESSURE AND TEMPERATURE GIVEN STAGNATION ENTROPY AND ENTHALPY.
C     THIS ROUTINE CALLS SUBROUTINE ECOM TO COMPUTE EQUILIBRIUM PRO-
C     PERTIES.
C
C     HS CONTAINS STAGNATION ENTHALPY
C     BLOCK(1-4) CONTAINS INITIAL VALUES OF P,T,S/R, AND H
C          FINAL P,T,S/R, AND H ARE STORED IN BLOCK(5-8)
C     NN IS AN ITERATION COUNT
C     1/Z, H/ZRT AND DENSITY STORED IN OOZ, HOZRT, AND RHO
```

# APPENDIX A

```
C
      DIMENSION OMEG(5,30,30),F(30),CAPM(30),A(10,30),L(30),
     1G(30,30),SMALE(30,30),X(30),CAPLAM(30,30),DHFO(30),YSTO(30)
C
      DIMENSION CP(5),BETA(5),AM(5),CODE(30),SHBL(8),REBL(8),STBL(8),
     1STSBL(8),NBTA(5)
C
      DIMENSION T(2),H(2),P(2),SR(2),BLOCK(8)
      COMMON OMEG,F,CAPM,A
      COMMON G,SMALE
      COMMON CONH,CONK,CONR,CONPRF,CONNO,N,M,L,NIT
      COMMON EPS1,EPS2,CAPLAM
      COMMON DHFO,AMC,IC1,YSTO
      COMMON P10,T10,US,RHO2,EPS5,NB,CP,BETA,AM,TP,DELT,IT,NBTA
      COMMON TR,RHOR
      COMMON FP,FT,ES
      COMMON TSTAG,RHOS
C
      COMMON SHBL,STBL,STSBL,REBL,SOR,X
C
      IR=0
      NN=1
C
C
C     SCHEME
C        INSIDE LOOP-  ITERATE ON T UNTIL ENTHALPY (H) CONVERGES
C        OUTSIDE LOOP- ITERATE ON P UNTIL ENTROPY (S/R) CONVERGES
C
C     FIRST PRESSURE CURVE
C
      SORS=BLOCK(3)
      P(1)=BLOCK(1)
      T(1)=BLOCK(2)
      SORS=BLOCK(3)
      H(1)=BLOCK(4)
      T(2)=T(1)+T(1)*FT
      CALL ECOM(T(2),P(1),OOZ,HOZRT,H(2),RHO)
      S=(H(2)-H(1))/(T(2)-T(1))
      T(1)=T(2)
      T(2)=T(1)+(HS-H(2))/S
      H(1)=H(2)
    5 CALL ECOM(T(2),P(1),OOZ,HOZRT,H(2),RHO)
      S=(H(2)-H(1))/(T(2)-T(1))
      T(1)=T(2)
      H(1)=H(2)
C
      REL=ABS(H(2)-HS)/HS
      IF(REL-ES)15,15,10
   15 REL=ABS((SORS-SOR)/SORS)
      IF(REL-ES)100,100,20
   10 T(2)=T(1)+(HS-H(2))/S
```

```
      GO TO 5
C
C     SECOND PRESSURE CURVE
C
   20 SR(1)=SOR
      SLAST=S
      TLAST=T(2)
      P(2)=P(1)+P(1)*FP
      T(1)=BLOCK(2)
   23 T(2)=T(1)+(HS-H(1))/SLAST
C
C     TWO DIMENSIONAL ITERATION LOOP
C
   24 CALL ECOM(T(2),P(2),OOZ,HOZRT,H(2),RHO)
      IF(IR)241,241,242
  241 SLAST=(H(2)-H(1))/(T(2)-T(1))
  242 H(1)=H(2)
      IR=0
      REL=ABS((HS-H(2))/HS)
      IF(REL-ES)30,30,25
C
C     H NON-CONVERGENT, CONTINUE ITERATION ON T
C
   25 T(1)=T(2)
      GO TO 23
C
C     H CONVERGES, TEST S/R
C
   30 SR(2)=SOR
      REL=ABS((SORS-SR(2))/SORS)
      IF(REL-ES)100,100,35
C
C     S/R NON-CONVERGENT - ADJUST P AND T AND CONTINUE ITERATIONS
C
   35 SP=(SR(2)-SR(1))/(P(2)-P(1))
      ST=(SR(2)-SR(1))/(T(2)-TLAST)
      P(1)=P(2)
      TLAST=T(2)
      T(1)=T(2)
      P(2)=P(1)+(SORS-SR(2))/SP
      T(2)=T(2)+(SORS-SR(2))/ST
      SR(1)=SR(2)
      NN=NN+1
      IR=1
      GO TO 24
C
C
C     S/R CONVERGES - STORE OUTPUT
C
  100 BLOCK(5)=P(2)
      BLOCK(6)=T(2)
```

```
      BLOCK(7)=SR(2)
      BLOCK(8)=H(2)
C
      RHO=RHO*1.E3
C
      RETURN
      END
```

```
$IBFTC ECOM
      SUBROUTINE ECOM(T,PSTO,OOZ,HOZRT,H,RHO)
C
C     SUBROUTINE WHICH, GIVEN A TEMPERATURE AND PRESSURE, COMPUTES
C     THE THERMODYNAMIC EQUILIBRIUM PROPERTIES OF A GAS DESCRIBED BY
C     THE INPUT.
C
C     T - TEMPERATURE
C     PSTO - PRESSURE
C     OOZ - 1/Z
C     HOZRT - H/ZRT
C     H - ENTHALPY
C     RHO - DENSITY
C
C     MOLE FRACTIONS (X(I)) STORED IN COMMON
C
      DIMENSION OMEG(5,30,30),F(30),CAPM(30),A(10,30),L(30),
     1G(30,30),SMALE(30,30),X(30),
     2E(30),Y(30),Q(30),CAPLAM(30,30),CAPFI(30),R(10,10),B(10),
     3TEMPS(10),BSUM(11,1),ABLOCK(11,11),PTEMP(30),ZETA(30),
     4ZETAPR(30),DHFO(30),ALAM(30),
     5YSTO(30),IPIVOT(11),INDEX(11,2),DQINT(30),QINT(30,30)
      DIMENSION CP(5),BETA(5),AM(5),SHBL(8),REBL(8),STBL(8),STSBL(8),
     1NBTA(5)
C
      COMMON OMEG,F,CAPM,A
      COMMON G,SMALE
      COMMON CONH,CONK,CONR
      COMMON  CONPRF , CONNO   , N       , M       , L       , NIT
      COMMON EPS1,EPS2,CAPLAM
      COMMON DHFO,AMC,IC1,YSTO
      COMMON P10,T10,US,RHO2,EPS5,NB,CP,BETA,AM,TP,DELT,IT,NBTA
      COMMON TR,RHOR
```

APPENDIX A

```
      COMMON FP,FT,ES
      COMMON TSTAG,RHOS
C
      COMMON SHBL,STBL,STSBL,REBL,SOR,X
C
      PI=3.14159
      C=2.99793E10
      NCOUNT=0
      LTEST=LTEST
      N2=N
      DO 5 I=1,N
    5 Y(I)=YSTO(I)
      P=PSTO
   34 TK=CONK*T
      RT=CONR*T
  346 YBAR=0.0
      DO 347 I=1,N
  347 YBAR=YBAR+Y(I)
      DO 40 I=1,N
      TEMP1=0
      LEND=L(I)
      DO 37 L1=1,LEND
      IF(F(I))31,35,31
   31 PROD=1.
      DO 33 IC=1,IC1
      IF(OMEG(IC,L1,I))32,33,32
   32 PROD=PROD*(1.-EXP(-CONH*C*OMEG(IC,L1,I)/TK))
   33 CONTINUE
      PART=(T/(CAPLAM(L1,I)*PROD))**F(I)
      GO TO 36
   35 PART=1.
   36 QINT(L1,I)=PART*G(L1,I)*EXP(-CONH*C*SMALE(L1,I)/TK)
   37 TEMP1=TEMP1+QINT(L1,I)
      Q(I)=(SQRT(2.*PI/CONH*TK/(CONH*CONNO)*CAPM(I))**3)*TK/CONPRF*TEMP1
      IF(Y(I)/YBAR)38,38,39
   38 CAPFI(I)=0
      GO TO 40
   39 CAPFI(I)=Y(I)*(ALOG(P/CONPRF)+ALOG(Y(I)/YBAR)-ALOG(Q(I))+DHFO(I)
     1/RT)
   40 CONTINUE
C
C     SENSE LIGHT 4 ON - DO NOT ITERATE
C     SENSE LIGHT 4 OFF - ITERATE
C
      CALL SLITET(4,JJ)
      GO TO (95,396),JJ
  396 DO 50 J=1,M
      DO 50 K=1,M
      R(K,J)=0.0
      B(J)=0.0
      DO 50 I=1,N
```

```
      B(J)=B(J)+A(J,I)*Y(I)
   50 R(K,J)=R(K,J)+A(J,I)*A(K,I)*Y(I)
C
C     SET UP MATRIX FOR SOLUTION OF EQUATIONS
C
      DO 60 J=1,M
      TEMPS(J)=0.0
      DO 55 I=1,N
   55 TEMPS(J)=TEMPS(J)+A(J,I)*CAPFI(I)
      BSUM(J,1)=B(J)+TEMPS(J)
C
C     CONSTANT TERMS IN BSUM BLOCK
C
      DO 56 K=1,M
      K1=K+1
   56 ABLOCK(J,K1)=R(K,J)
C
C     PI TERMS IN ABLOCK IN COLUMNS 2 THROUGH N+1
C
   60 ABLOCK(J,1)=B(J)
C
C     (X/Y) TERMS IN FIRST COLUMN
C
      M1=M+1
      ABLOCK(M1,1)=0.0
      DO 61 K=1,M1
      K1=K+1
   61 ABLOCK(M1,K1)=B(K)
      BSUM(M1,1)=0.0
      DO 62 I=1,N
   62 BSUM(M1,1)=BSUM(M1,1)+CAPFI(I)
C
C     MATINV EXPECTS AN M+1 BY M+1 MATRIX
C
      CALL MATINV(ABLOCK(1,1),M1,BSUM(1,1),1,DETERM,IPIVOT,INDEX,11,0)
C
C     RETURN WITH ANSWERS IN BSUM
C
      ZETAP=BSUM(1,1)*YBAR
      ZERO=0.
      NEG=0.0
      DO 70 I=1,N
      PTEMP(I)=0.0
      DO 65 J=1,M
      J1=J+1
   65 PTEMP(I)=PTEMP(I)+BSUM(J1,1)*A(J,I)*Y(I)
      ZETA(I)=-CAPFI(I)+Y(I)*BSUM(1,1)+PTEMP(I)
C
C     TEST FOR NEGATIVE OR ZERO ZETA
C
   68 IF(ZETA(I))69,695,70
```

```
   69 PIECE=-Y(I)/(ZETA(I)-Y(I))
      IF(PIECE)691,692,691
  691 NEG=NEG+1
      ALAM(NEG)=PIECE
      GO TO 70
  692 Y(I)=0
      ZERO=1.
      GO TO 70
  695 IF(Y(I))69,70,69
   70 CONTINUE
C
C     FIND GREATEST NEGATIVE ZETA-Y
C
      IF(ZERO)700,700,698
  698 IF(NCOUNT-NIT)699,100,100
  699 NCOUNT=NCOUNT+1
      GO TO 346
  700 IF(NEG-1)78,71,73
   71 ALAMPR=.999999*ALAM(1)
      GO TO 745
   73 ARG1=ALAM(1)
      DO 74 I=2,NEG
   72 ARG2=ALAM(I)
      ARG1=AMIN1(ARG1,ARG2)
   74 CONTINUE
      ALAMPR=.999999*ARG1
  745 IIC=0
   75 ZETAP=0
      DO 76 I=1,N
      ZETAPR(I)=Y(I)+ALAMPR*(ZETA(I)-Y(I))
   76 ZETAP=ZETAP+ZETAPR(I)
      DLAM=0
      DO 77 I=1,N
      IF(ZETAPR(I)/ZETAP)77,77,765
  765 DLAM=DLAM+(ZETA(I)-Y(I))*(ALOG(P/CONPRF)-ALOG(Q(I))+DHFO(I)/RT+ALO
     1G(ZETAPR(I)/ZETAP))
   77 CONTINUE
      IF(DLAM)81,81,80
   80 IF(IIC-3)805,81,81
  805 IIC=IIC+1
      ALAMPR=ALAMPR*.9
      GO TO 75
   78 ALAMPR=1.
      GO TO 745
C
C     CONVERGENCE TEST FOR Y(I)S
C
   81 IF(ALAMPR-.50)83,815,815
  815 DO 82 I=1,N
      IF(ZETAPR(I))813,816,813
  813 REL=Y(I)-ZETAPR(I)
```

```
      IF(ABS(REL)-EPS1)818,818,83
  818 REL=ZETAPR(I)/Y(I)-1.
      IF(ABS(REL)-EPS2)82,82,83
  816 IF(Y(I))817,82,817
  817 GO TO 83
   82 CONTINUE
C
C     Y(I)S CONVERGE
C
      DO 800 I=1,N
  800 Y(I)=ZETAPR(I)
      GO TO 95
C
C     NON-CONVERGENCE OF Y(I)S
C
   83 NCOUNT=NCOUNT+1
      IF(NCOUNT-NIT)84,100,100
   84 DO 85 I=1,N
   85 Y(I)=ZETAPR(I)
C
C     REPEAT WITH NEW Y(I)S AND NO. OF ITERATIONS LESS THAN NIT
C
      GO TO 346
   95 DO 201 I=1,N
  201 X(I)=Y(I)*CAPM(I)
      YBAR=0.0
      CAPMI=0
      DO 2026 I=1,N
      YBAR=YBAR+Y(I)
 2026 CAPMI=CAPMI+X(I)/CAPM(I)
      CAPMI=1.0/CAPMI
      Z=AMC/CAPMI
      ESUM=0
      DO 2029 I=1,N
      QSUM=0
      DQINT(I)=0
      LEND=L(I)
      DO 2028 L1=1,LEND
      SUM=0
      DO 2027 IC=1,IC1
      HOOTK=CONH*C*OMEG(IC,L1,I)/TK
      IF(OMEG(IC,L1,I))2000,2027,2000
 2000 SUM=SUM+HOOTK/(EXP(HOOTK)-1.)
 2027 CONTINUE
      DQINT(I)=DQINT(I)+QINT(L1,I)*(F(I)/T*(1.+SUM)+SMALE(L1,I)*CONH*C
     1/(TK*T))
 2028 QSUM=QSUM+QINT(L1,I)
      E(I)=1./CAPM(I)*(1.5*RT+RT*T/QSUM*DQINT(I)+DHFO(I))
 2029 ESUM=ESUM+X(I)*E(I)
      HOZRT=CAPMI*ESUM/RT+1.0
      H=HOZRT*CONR*T*Z/AMC
```

```
      TK=T*CONK
      FSUM=0
      DO 2040 I=1,N
 2033 IF(Y(I)/YBAR)2034,2034,2035
 2034 CAPFI(I)=0
      GO TO 2040
 2035 CAPFI(I)=Y(I)*(ALOG(P/CONPRF)+ALOG(Y(I)/YBAR)-ALOG(Q(I))+DHFO(I)
     1/RT)
 2040 FSUM=FSUM+CAPFI(I)
      SOZR=HOZRT-CAPMI*FSUM
      SOR=SOZR*Z
      RHO=P*CAPMI/RT
      U=CAPX+.43429*ALOG(273.16/(Z*T))
      OOZ=1.0/Z
      DO 300 I=1,N
  300 X(I)=X(I)*CAPMI/CAPM(I)
      RETURN
  100 WRITE(6,5000)
 5000 FORMAT(1H0,25H THIS CASE NON-CONVERGENT)
      CALL EXIT
      END
```

```
$IBMAP SYMBOL  150
*
*         SUBROUTINE WHICH DEFINES INPUT AND ITS STORAGE FOR THE
*         LOADING ROUTINE (PW-LOAD)
*
       ENTRY    SYMBOL
SYMBOL BCI      1,OMEG
       PZE      OMEG
       BCI      1,F
       PZE      F
       BCI      1,CAPM
       PZE      CAPM
       BCI      1,A
       PZE      A
       BCI      1,G
       PZE      G
       BCI      1,SMALE
       PZE      SMALE
       BCI      1,CONH
       PZE      CONH
```

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```
BCI     1,CONK
PZE     CONK
BCI     1,CONR
PZE     CONR
BCI     1,CONPRF
PZE     CONPRF
BCI     1,CONNO
PZE     CONNO
BCI     1,N
PZE     N
BCI     1,M
PZE     M
BCI     1,L
PZE     L
BCI     1,NIT
PZE     NIT
BCI     1,EPS1
PZE     EPS1
BCI     1,EPS2
PZE     EPS2
BCI     1,CAPLAM
PZE     CAPLAM
BCI     1,DHFO
PZE     DHFO
BCI     1,AMC
PZE     AMC
BCI     1,IC1
PZE     IC1
BCI     1,YSTO
PZE     YSTO
BCI     1,P10
PZE     P10
BCI     1,T10
PZE     T10
BCI     1,US
PZE     US
BCI     1,RHO2
PZE     RHO2
BCI     1,EPS5
PZE     EPS5
BCI     1,NB
PZE     NB
BCI     1,CP
PZE     CP
BCI     1,BETA
PZE     BETA
BCI     1,AM
PZE     AM
BCI     1,TP
PZE     TP
BCI     1,DELT
```

APPENDIX A

```
          PZE     DELT
          BCI     1,IT
          PZE     IT
          BCI     1,NBTA
          PZE     NBTA
          BCI     1,TR
          PZE     TR
          BCI     1,RHOR
          PZE     RHOR
          BCI     1,FP
          PZE     FP
          BCI     1,FT
          PZE     FT
          BCI     1,ES
          PZE     ES
          BCI     1,TSTAG
          PZE     TSTAG
          BCI     1,RHOS
          PZE     RHOS
          HTR     **
//        CONTRL  //
OMEG      COMMON  4500
F         COMMON  30
CAPM      COMMON  30
A         COMMON  300
G         COMMON  900
SMALE     COMMON  900
CONH      COMMON  1
CONK      COMMON  1
CONR      COMMON  1
CONPRF    COMMON  1
CONNO     COMMON  1
N         COMMON  1
M         COMMON  1
L         COMMON  30
NIT       COMMON  1
EPS1      COMMON  1
EPS2      COMMON  1
CAPLAM    COMMON  900
DHF0      COMMON  30
AMC       COMMON  1
IC1       COMMON  1
YSTO      COMMON  30
P10       COMMON  1
T10       COMMON  1
US        COMMON  1
RHO2      COMMON  1
EPS5      COMMON  1
NB        COMMON  1
CP        COMMON  5
BETA      COMMON  5
```

```
AM      COMMON  5
TP      COMMON  1
DELT    COMMON  1
IT      COMMON  1
NBTA    COMMON  5
TR      COMMON  1
RHOR    COMMON  1
FP      COMMON  1
FT      COMMON  1
ES      COMMON  1
TSTAG   COMMON  1
RHOS    COMMON  1
        END
```

# APPENDIX B

## PROGRAM INPUT

The input necessary to utilize the included program is presented in this appendix. The species in the undissociated free stream must be assigned a value of the subscript $p$ beginning with unity. Similarly, the species to be considered (atoms, molecules, ions, or electrons) in the dissociated mixture must be assigned a value of the subscript $i$, whereas each elemental particle (atomic particle or electron) is given a value of the subscript $j$. Electrons, if considered as a species, must be assigned the value of 1 for the subscript $i$. The program as it presently stands is limited to the consideration of ten elements with five species in the undissociated free stream and thirty species in the dissociated mixture. The capacity of the program with regard to the number of species considered is easily increased by changing pertinent dimension statements.

A description of additional input required by the program is given in the following table:

APPENDIX B

| Input | Program symbol | Description | Unit |
|---|---|---|---|
| Thermodynamic input | | | |
| $\omega_{ilc}$ | ∅MEG | cth characteristic vibrational frequency of $l$th electronic level of ith species ($\omega_{ilc} = \omega_e - \omega_e x_e$) | $cm^{-1}$ |
| $y_i$ | YST∅ | Initial guess, not equal to zero, for mole number of ith species satisfying $b_j = \sum a_{ij} y_i$ where $b_j = \frac{1}{M_1} \sum_p a_{pj}\beta_p$, the product $a_{pj}\beta_p$ being evaluated in the free stream | |
| $f_i$ | F | Zero if species is atom or atomic ion; unity if species is molecule or molecular ion | |
| $M_i$ | CAPM | Molecular weight of ith species | grams/mole |
| $a_{ij}$ | A | Number of jth atoms in ith species | |
| $g_{il}$ | G | Degeneracy of $l$th electronic energy level of ith species | |
| $\epsilon_{il}$ | SMALE | Excitation energy of $l$th electronic level in ith species | $cm^{-1}$ |
| $h$ | C∅NH | Planck's constant | erg-sec |
| $k$ | C∅NK | Boltzmann constant | ergs/$^{\circ}$K |
| $\mathcal{R}$ | C∅NR | Universal gas constant | ergs/mole-$^{\circ}$K |
| $p_{ref}$ | C∅NPRF | Reference pressure | dynes/$cm^2$ |
| $N_A$ | C∅NN∅ | Avogadro's number | particles/mole |
| $n$ | N | Number of species $i$ | |
| $m$ | M | Number of types of atoms $j$ appearing in mixture (exclude ions) | |
| $l_i$ | L | Number of electronic energy levels considered in ith species | |
| $N_{it}$ | NIT | Maximum number of iterations in equilibrium subroutine; normally 100 | |
| $\epsilon_1$ | EPS1 | Convergence criterion for absolute test of $y_i$ in equilibrium subroutine; normally $10^{-7}$ | |
| $\epsilon_2$ | EPS2 | Convergence criterion for relative test on $y_i$ in equilibrium subroutine; normally $\epsilon_2 = 10$ and is not used | |
| $\Lambda_{il}$ | CAPLAM | Product of symmetry number and characteristic rotational temperature of $l$th electronic level of ith species | $^{\circ}$K |

| | | | |
|---|---|---|---|
| $\left(\Delta H_{fo}^{o}\right)_i$ | ΔHFO | Standard heat of formation at $0^{o}$ K of ith species | ergs/mole |
| M1 | AMC | Molecular weight of free-stream gas at $300^{o}$ K | grams/mole |
| c | IC1 | Maximum number of c's for $l$th level of ith species (refers to $\omega_{ilc}$ for triatomic species) | |
| $\beta_p$ | BETA | Mole fraction of pth species in free-stream gas at $300^{o}$ K | |
| $M_p$ | AM | Molecular weight of pth species in free stream | grams/mole |
| $\Delta T$ | DELT | Temperature increment for incident and reflected shock solutions; normally $10^{o}$ K | $^{o}$K |
| $I_t$ | IT | Option code for additional iteration on temperature in incident and reflected shock subroutines; normally 3 | |
| $n_{\beta p}$ | NBTA | Value of i assigned to pth species in dissociated mixture | |
| $f_p$ | FP | Fraction required for incrementing pressure in stagnation point solution; normally $5 \times 10^{-5}$ | |
| $f_T$ | FT | Fraction required for incrementing temperature in stagnation point solution; normally $5 \times 10^{-5}$ | |
| $\epsilon_{st}$ | ES | Convergence criterion for entropy and enthalpy in stagnation point solution; normally $10^{-4}$ | |
| | | Flow input | |
| $p_1$ | P10 | Free-stream pressure | atmospheres |
| $T_1$ | T10 | Free-stream temperature | $^{o}$K |
| $U_s$ | US | Incident shock speed | feet/sec |
| $\rho_{2e}$ | RHØ2 | Estimated density behind incident shock | Nondimensional |
| $\epsilon_5$ | EPS5 | Convergence criterion for $\rho$ in incident and reflected shock iterations; normally $10^{-3}$ | |
| $T_{2e}$ | TP | Estimated temperature behind incident shock | $^{o}$K |
| $T_{5e}$ | TR | Estimated temperature behind reflected shock | $^{o}$K |
| $\rho_{5e}$ | RHØR | Estimated density behind reflected shock | Nondimensional |
| $T_{3e}$ | TSTAG | Estimated temperature behind standing shock | $^{o}$K |
| $\rho_{3e}$ | RHØS | Estimated density behind standing shock | Nondimensional |

## APPENDIX B

Once the input has been determined for a given initial mixture and species to be considered, duplication for solutions with varying flow conditions, such as initial pressure, temperature, and shock speed, is not necessary. Computations involving these variations require only the respecification of quantities given in the foregoing table under Flow input. Similarly, if it is desired to determine the effect on the solution of one of the species constants, such as the heat of formation of that species, it is necessary to change only that value. However, if changes in the mole fractions of the initial mixture are made, it is necessary to reestimate values of $y_i$ to insure that the charge and mass balance constraints are satisfied.

### Input Loading and Comments

The input is loaded by a symbolic loader routine, LOAD. Subroutine SYMBOL describes the input, giving its symbolic name, number of locations required, and location in COMMON. Any suitable routine may be used to enter the input by appropriately modifying statement 1 in the main program.

For purposes of output, $n + 1$ cards are read into the program in front of the data to identify the $n$ species in the shock processed mixture. Card 1 contains the number $n$ (cols. 1 to 3) and cards 2 through $n + 1$ contain alphabetic identification of the species (cols. 1 to 6) - for example, N2O, O2, and $A^{++}$.

After all the data are loaded, the program reads one card (cols. 1 to 3) containing a numeric code for computing option desired:

0 - incident shock only

1 - incident and reflected shocks

2 - incident shock and in-flight stagnation conditions

3 - incident and reflected shocks, and in-flight stagnation conditions

4 - incident shock, and shock-tube stagnation conditions

5 - incident and reflected shocks, and shock-tube stagnation conditions

6 - incident shock, shock-tube and in-flight stagnation conditions

7 - incident and reflected shocks, shock-tube and in-flight stagnation conditions

The program also uses a routine MATINV to solve a matrix equation, $AX = B$, where $A$ is a square coefficient matrix and $B$ is a matrix of constant vectors. Reference to this routine is found in subroutine ECOM following statement 62.

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The calling sequence of this routine is shown and briefly described as follows in order to allow replacement by a similar routine, if necessary:

CALL MATINV (ABLOCK (1,1), M1, BSUM (1,1), 1, DETERM, IPIVOT, INDEX, 11, 0)

ABLOCK - the first location of two-dimensional array of matrix A

M1 - the location of order of A, $1 \leqq M1 \leqq 11$

BSUM - the first location of two-dimensional array of constant vectors B

1 - the number of column vectors

DETERM - gives value of determinant (not used)

IPIVOT - temporary storage

INDEX - temporary storage

11 - the maximum order of A

0 - a factor used in computing determinant

At the return to the calling program, x is stored at BSUM.

### Sample Output

A typical program output for air is given herein. p is in standard atmospheres, $U_s$, $U_r$, $u_2$ are in ft/sec, T is in $^{\circ}$K, and $\rho$ is nondimensionalized by $\bar{\rho} = 1.936(10^{-3})\frac{\text{slugs}}{\text{ft}^3} = 10^{-3}\,\frac{\text{grams}}{\text{cc}}$. Other quantities are nondimensionalized with the exception of the stagnation enthalpies which are in $\text{cm}^2/\text{sec}^2$. The sample computer print-out is as follows:

INPUT FCR INCIDENT SHCCK

RHC-1 = C.12724344E C1   P-1 = C.39999999E C1   US= 0.3CCCCOCCE C5   T-1 = 0.3CCOCCCOE C3

BETA

| N2 | CO2 | A |
|---|---|---|
| 0.7600CCCCE CC | C.11CCCOCCE-OC | C.13CCCCCCE-CC |

ASSUMEC RHC= C.09999999E C2

CUTPUT

U2 = C.27657165E C5                NC. CF MAJOR ITERATICNS = 5

| P | RHC | 1/Z | H/ZRT | S/R | T | M1 |
|---|---|---|---|---|---|---|
| 0.96904850E C3 | C.16294269E 02 | C.56274641E CO | C.67112346E C1 | C.431167C1E 02 | C.12776147E 05 | C.31326C90E C2 |

| FINAL X FRCM ITERATICN | SPECIES |
|---|---|
| C.72836C74E-C2 | E- |
| C.6273C5C8E CC | N |
| C.369513C2E-C2 | N+ |
| 0.11379162E-CC | O |
| C.38751387E-C3 | C+ |
| C.51C65551E-01 | C |
| C.17867831E-C2 | C+ |
| C.727C0819E-C1 | A |
| C.45645799E-C3 | A+ |
| C.1C586238E-CC | N2 |
| 0.54371160E-C3 | N2+ |
| C.1C67344CE-C3 | O2 |
| C.5563431CE-C2 | NC |
| C.41405477E-C3 | NC+ |
| 0.12752569E-C4 | C2 |
| C.34333257E-C2 | CO |
| C.559CC569E-C2 | CN |
| C.1C381966E-C5 | CO2 |

SHCCK TUBE STAGNATICN PCINT CATA IS CCMPUTEC FROM THE FOLLOWING STANDING SHCCK CATA

| P | RHC | 1/Z | H/ZRT | S/R | T | M1 |
|---|---|---|---|---|---|---|
| C.102237C8E C5 | C.85691168E C2 | C.48674144E-CC | C.617823C9E C1 | C.46117C31E C2 | 0.22169056E C5 | C.31326C90E C2 |

SHCCK TUBE STAGNATICN PCINT ENTHALPY =    C.75973347E 12

CUTPUT

PRESSURE = C.11359996E C5     TEMPERATURE = C.22522939E C5     NO. OF MAJOR ITERATIONS = 4

1/Z = C.486257C4E-CC     H/ZRT = C.61796464E C1     RHC = C.93622503E C2     S/R = 0.46117213E C2     H = C.75973626E 12

| FINAL X FRCM ITERATICN | SPECIES |
|---|---|
| C.55171687E-C1 | E- |
| C.66930937E CC | N |
| C.38569783E-C1 | N+ |
| 0.99941716E-01 | O |
| C.38991915E-C2 | O+ |
| C.47304658E-C1 | C |
| C.4622861CE-C2 | C+ |
| 0.56771533E-C1 | A |
| C.64419228E-C2 | A+ |
| C.12483915E-C1 | N2 |
| C.1192C340E-C2 | N2+ |
| C.10C52688E-C3 | O2 |
| C.21869799E-C2 | NC |
| C.44622724E-C3 | NC+ |
| C.34161465E-C5 | C2 |
| 0.30234C67E-C3 | CO |
| C.12518514E-C2 | CN |
| C.62CC5485E-C7 | CO2 |

# APPENDIX B

```
REFLECTED SHOCK

   ASSUMED RHO = 0.59999999E 02


OUTPUT

U-R= 0.51858532E 04                    NO. OF MAJOR ITERATIONS =  5

        P             RHO              1/Z              H/ZRT            S/R              T                M1

  0.14539860E 05   0.10319477E 03   0.47120168E-00   0.62550054E 01   0.47700314E 02   0.25344627E 05   0.31326090E 02

FINAL X FROM ITERATION     SPECIES

  0.77387073E-01           E-
  0.64283480E 00           N
  0.55606787E-01           N+
  0.95394575E-01           O
  0.61307509E-02           O+
  0.45581391E-01           C
  0.54365706E-02           C+
  0.52483761E-01           A
  0.87725917E-02           A+
  0.66348217E-02           N2
  0.10277247E-02           N2+
  0.78229235E-04           O2
  0.14052661E-02           NO
  0.41299297E-03           NO+
  0.17578935E-05           C2
  0.16513067E-03           CO
  0.64584481E-03           CN
  0.23657988E-07           CO2



  IN FLIGHT STAGNATION POINT DATA IS COMPUTED FROM THE INCIDENT SHOCK OUTPUT

STAGNATION ENTHALPY = 0.40696681E 12      STAGNATION ENTROPY = 0.43116701E 02



OUTPUT

    PRESSURE = 0.10119144E 04     TEMPERATURE = 0.12854929E 05                    NO. OF MAJOR ITERATIONS =  3

1/Z = 0.56179306E 00     H/ZRT = 0.67005274E 01     RHO = 0.16882119E 02     S/R = 0.43114194E 02     H = 0.40695124E 12

FINAL X FROM ITERATION     SPECIES

  0.74532434E-02           E-
  0.62900783E 00           N
  0.38074829E-02           N+
  0.11364757E-00           O
  0.39727855E-03           O+
  0.51040160E-01           C
  0.18044082E-02           C+
  0.72560759E-01           A
  0.47259831E-03           A+
  0.10422159E-00           N2
  0.55593066E-03           N2+
  0.10777555E-03           O2
  0.55677062E-02           NO
  0.41558252E-03           NO+
  0.12763625E-04           C2
  0.33497790E-02           CO
  0.55765794E-02           CN
  0.10233709E-05           CO2
```

## APPENDIX C

## PHYSICAL CONSTANTS

The physical constants required by the computer program for use with the 27 chemical species are as follows:

| | |
|---|---|
| Planck's constant, h, erg-sec . . . . . . . . . . . . . . . . . . . . | $6.62517 \times 10^{-27}$ |
| Boltzmann constant, k, ergs/°K . . . . . . . . . . . . . . . . . . . | $1.38044 \times 10^{-16}$ |
| Universal gas constant, $\mathcal{R}$, ergs/mole-°K . . . . . . . . . . . . . | $8.31469 \times 10^{7}$ |
| Reference pressure, $p_{ref}$, dynes/cm$^2$ . . . . . . . . . . . . . . . . | $1.01325 \times 10^{6}$ |
| Avogadro's number, $N_A$, particles/mole . . . . . . . . . . . . . . | $6.02322 \times 10^{23}$ |
| Speed of light, c, cm/sec . . . . . . . . . . . . . . . . . . . . . | $2.99793 \times 10^{10}$ |

The molecular weight and heat of formation of the chemical species are given in the following table:

| Species | i | $M_i$ | $f_i$ | $\left(\Delta H_{fo}^{o}\right)_i$ |
|---|---|---|---|---|
| $e^-$ | 1* | $5.4847 \times 10^{-4}$ | 0 | 0 |
| N | | 14.008 | 0 | $4.70729 \times 10^{12}$ |
| $N^+$ | | 14.007 | 0 | 18.72607 |
| $N^{++}$ | | 14.007 | 0 | 47.28829 |
| O | | 16.000 | 0 | 2.46741 |
| $O^+$ | | 15.999 | 0 | 15.60389 |
| $O^{++}$ | | 15.999 | 0 | 49.47996 |
| $O^-$ | | 16.001 | 0 | 1.05410 |
| C | | 12.011 | 0 | 7.11238 |
| $C^+$ | | 12.010 | 0 | 17.97182 |
| $C^{++}$ | | 12.010 | 0 | 41.49225 |
| $C^-$ | | 12.012 | 0 | 5.89944 |
| A | | 39.944 | 0 | 0 |
| $A^+$ | | 39.943 | 0 | 15.20235 |
| $A^{++}$ | | 39.943 | 0 | 41.85170 |
| $N_2$ | | 28.016 | 1 | 0 |
| $N_2^+$ | | 28.015 | 1 | 15.03336 |
| $O_2$ | | 32.000 | 1 | 0 |
| $O_2^+$ | | 31.999 | 1 | 11.62808 |
| $O_2^-$ | | 32.001 | 1 | -.96232 |
| NO | | 30.008 | 1 | .89860 |
| $NO^+$ | | 30.007 | 1 | 9.82403 |
| CO | | 28.011 | 1 | -1.13813 |
| $CO^+$ | | 28.010 | 1 | 12.38367 |
| CN | | 26.019 | 1 | 4.56056 |
| $CO_2$ | | 44.011 | 1 | -3.93146 |
| $N_2O$ | | 44.016 | 1 | .84973 |

*If electrons are included as a species, they must be assigned a value of 1 for the subscript i; otherwise values of i may be assigned to species as desired.

## APPENDIX C

The number of jth particles in ith species is shown in the following table:

| Species | i | †$a_{ij}$ for - N | O | C | A | $e^-$ |
|---|---|---|---|---|---|---|
| $e^-$ | 1* | 0 | 0 | 0 | 0 | +1 |
| N | | 1 | 0 | 0 | 0 | 0 |
| $N^+$ | | 1 | 0 | 0 | 0 | -1 |
| $N^{++}$ | | 1 | 0 | 0 | 0 | -2 |
| O | | 0 | 1 | 0 | 0 | 0 |
| $O^+$ | | 0 | 1 | 0 | 0 | -1 |
| $O^{++}$ | | 0 | 1 | 0 | 0 | -2 |
| $O^-$ | | 0 | 1 | 0 | 0 | +1 |
| C | | 0 | 0 | 1 | 0 | 0 |
| $C^+$ | | 0 | 0 | 1 | 0 | -1 |
| $C^{++}$ | | 0 | 0 | 1 | 0 | -2 |
| $C^-$ | | 0 | 0 | 1 | 0 | +1 |
| A | | 0 | 0 | 0 | 1 | 0 |
| $A^+$ | | 0 | 0 | 0 | 1 | -1 |
| $A^{++}$ | | 0 | 0 | 0 | 1 | -2 |
| $N_2$ | | 2 | 0 | 0 | 0 | 0 |
| $N_2^+$ | | 2 | 0 | 0 | 0 | -1 |
| $O_2$ | | 0 | 2 | 0 | 0 | 0 |
| $O_2^+$ | | 0 | 2 | 0 | 0 | -1 |
| $O_2^-$ | | 0 | 2 | 0 | 0 | +1 |
| NO | | 1 | 1 | 0 | 0 | 0 |
| $NO^+$ | | 1 | 1 | 0 | 0 | -1 |
| CO | | 0 | 1 | 1 | 0 | 0 |
| $CO^+$ | | 0 | 1 | 1 | 0 | -1 |
| CN | | 1 | 0 | 1 | 0 | 0 |
| $CO_2$ | | 0 | 2 | 1 | 0 | 0 |
| $N_2O$ | | 2 | 1 | 0 | 0 | 0 |

†Values of j for the elements shown may be assigned as desired.

*If electrons are included as a species, they must be assigned a value of 1 for the subscript i; otherwise values of i may be assigned to species as desired.

# APPENDIX C

Spectroscopic constants and quantities for the 27 species are as follows (values of $\omega_{ilc}$ and $\Lambda_{il}$ being listed only where required):

| Species | i | $l$ | $g_{il}$ | $\epsilon_{il}$ |
|---|---|---|---|---|
| $e^-$ | 1* | 1 | 2 | 0 |
| N | | 1 | 4 | 0 |
| | | 2 | 10 | 19225 |
| | | 3 | 6 | 28840 |
| | | 4 | 12 | 83330 |
| | | 5 | 6 | 86180 |
| | | 6 | 12 | 88140 |
| | | 7 | 2 | 93582 |
| | | 8 | 20 | 94800 |
| | | 9 | 12 | 95500 |
| | | 10 | 4 | 96752 |
| | | 11 | 10 | 96810 |
| | | 12 | 6 | 97800 |
| | | 13 | 10 | 99660 |
| | | 14 | 18 | 104000 |
| | | 15 | 34 | 104700 |
| | | 16 | 56 | 105000 |
| | | 17 | 22 | 106600 |
| | | 18 | 16 | 107200 |
| | | 19 | 16 | 107600 |
| | | 20 | 54 | 109600 |
| | | 21 | 12 | 109860 |
| | | 22 | 106 | 110350 |
| | | 23 | 132 | 111600 |
| | | 24 | 136 | 112200 |
| | | 25 | 6 | 112310 |
| | | 26 | 68 | 112820 |
| | | 27 | 30 | 112910 |
| | | 28 | 2 | 113600 |
| | | 29 | 10 | 113900 |
| | | 30 | 14 | 117000 |

| Species | i | $l$ | $g_{il}$ | $\epsilon_{il}$ |
|---|---|---|---|---|
| $N^+$ | | 1 | 9 | 0 |
| | | 2 | 5 | 15316 |
| | | 3 | 1 | 32687 |
| | | 4 | 5 | 47168 |
| | | 5 | 15 | 92245 |
| | | 6 | 9 | 109220 |
| | | 7 | 5 | 144189 |
| | | 8 | 12 | 149000 |
| | | 9 | 3 | 155130 |
| | | 10 | 3 | 164612 |
| | | 11 | 18 | 166650 |
| | | 12 | 3 | 168893 |
| | | 13 | 9 | 170620 |
| | | 14 | 5 | 174212 |
| | | 15 | 1 | 178274 |
| | | 16 | 41 | 187090 |
| | | 17 | 16 | 189100 |
| | | 18 | 3 | 190121 |
| | | 19 | 12 | 197200 |
| | | 20 | 30 | 203000 |
| | | 21 | 21 | 205700 |
| | | 22 | 153 | 210500 |
| | | 23 | 12 | 214828 |
| | | 24 | 12 | 218000 |
| | | 25 | 546 | 220500 |
| | | 26 | 37 | 223000 |
| | | 27 | 15 | 226000 |
| | | 28 | 15 | 228000 |
| | | 29 | 14 | 230300 |
| | | 30 | 5 | 234250 |

| Species | i | $l$ | $g_{il}$ | $\epsilon_{il}$ |
|---|---|---|---|---|
| $N^{++}$ | | 1 | 6 | 0 |
| | | 2 | 12 | 57280 |
| | | 3 | 10 | 101026 |
| | | 4 | 2 | 131044 |
| | | 5 | 6 | 145920 |
| | | 6 | 4 | 186802 |
| | | 7 | 10 | 203078 |
| | | 8 | 2 | 221302 |
| | | 9 | 6 | 230307 |
| | | 10 | 6 | 245690 |
| | | 11 | 10 | 267242 |
| | | 12 | 12 | 287650 |
| | | 13 | 6 | 297210 |
| | | 14 | 2 | 301088 |
| | | 15 | 32 | 310500 |
| | | 16 | 4 | 314224 |
| | | 17 | 22 | 317550 |
| | | 18 | 14 | 320288 |
| | | 19 | 10 | 321040 |
| | | 20 | 30 | 329000 |
| | | 21 | 22 | 333300 |
| | | 22 | 22 | 336290 |
| | | 23 | 20 | 339550 |
| | | 24 | 48 | 343000 |
| | | 25 | 24 | 348000 |
| | | 26 | 32 | 364000 |
| | | 27 | 12 | 368620 |
| | | 28 | 22 | 374000 |
| | | 29 | 52 | 379000 |
| | | 30 | 2 | 380700 |

*If electrons are included as a species, they must be assigned a value of 1 for the subscript i; otherwise values of i may be assigned to species as desired.

# APPENDIX C

| Species | i | $l$ | $g_{il}$ | $\epsilon_{il}$ |
|---|---|---|---|---|
| O | | 1 | 5 | 0 |
| | | 2 | 3 | 159 |
| | | 3 | 1 | 227 |
| | | 4 | 5 | 15868 |
| | | 5 | 1 | 33792 |
| | | 6 | 5 | 73768 |
| | | 7 | 3 | 76795 |
| | | 8 | 15 | 86630 |
| | | 9 | 9 | 88630 |
| | | 10 | 5 | 95476 |
| | | 11 | 3 | 96226 |
| | | 12 | 36 | 97420 |
| | | 13 | 15 | 97488 |
| | | 14 | 15 | 99094 |
| | | 15 | 9 | 99680 |
| | | 16 | 9 | 100000 |
| | | 17 | 15 | 101140 |
| | | 18 | 5 | 102116 |
| | | 19 | 3 | 102412 |
| | | 20 | 5 | 102662 |
| | | 21 | 25 | 102865 |
| | | 22 | 15 | 102908 |
| | | 23 | 9 | 103869 |
| | | 24 | 15 | 104000 |
| | | 25 | 25 | 105385 |
| | | 26 | 15 | 105408 |
| | | 27 | 56 | 106000 |
| | | 28 | 56 | 107000 |

| Species | i | $l$ | $g_{il}$ | $\epsilon_{il}$ |
|---|---|---|---|---|
| $O^+$ | | 1 | 4 | 0 |
| | | 2 | 10 | 26820 |
| | | 3 | 6 | 40465 |
| | | 4 | 12 | 120000 |
| | | 5 | 10 | 165990 |
| | | 6 | 12 | 185400 |
| | | 7 | 6 | 189000 |
| | | 8 | 2 | 195710 |
| | | 9 | 2 | 203942 |
| | | 10 | 42 | 207600 |
| | | 11 | 26 | 212800 |
| | | 12 | 2 | 226851 |
| | | 13 | 24 | 230000 |
| | | 14 | 80 | 232700 |
| | | 15 | 16 | 233900 |
| | | 16 | 18 | 239600 |
| | | 17 | 40 | 245500 |
| | | 18 | 20 | 248000 |
| | | 19 | 6 | 250300 |
| | | 20 | 32 | 251900 |
| | | 21 | 44 | 254000 |
| | | 22 | 84 | 255500 |
| | | 23 | 116 | 256000 |
| | | 24 | 18 | 258100 |
| | | 25 | 10 | 259300 |
| | | 26 | 72 | 261500 |
| | | 27 | 166 | 265500 |
| | | 28 | 134 | 270000 |
| | | 29 | 142 | 276500 |
| | | 30 | 24 | 283000 |

| Species | i | $l$ | $g_{il}$ | $\epsilon_{il}$ |
|---|---|---|---|---|
| $O^{++}$ | | 1 | 9 | 0 |
| | | 2 | 5 | 20271 |
| | | 3 | 1 | 43184 |
| | | 4 | 5 | 60312 |
| | | 5 | 15 | 120050 |
| | | 6 | 9 | 142383 |
| | | 7 | 5 | 187049 |
| | | 8 | 3 | 197087 |
| | | 9 | 3 | 210459 |
| | | 10 | 12 | 270000 |
| | | 11 | 9 | 283900 |
| | | 12 | 26 | 294000 |
| | | 13 | 14 | 303000 |
| | | 14 | 1 | 313801 |
| | | 15 | 50 | 327000 |
| | | 16 | 10 | 332000 |
| | | 17 | 15 | 338700 |
| | | 18 | 1 | 343303 |
| | | 19 | 9 | 350200 |
| | | 20 | 12 | 357500 |
| | | 21 | 46 | 365000 |
| | | 22 | 48 | 370500 |
| | | 23 | 158 | 380000 |
| | | 24 | 62 | 394000 |
| | | 25 | 90 | 398000 |
| | | 26 | 558 | 403400 |
| | | 27 | 72 | 425000 |
| | | 28 | 311 | 430000 |
| | | 29 | 48 | 438000 |
| | | 30 | 15 | 442710 |

## APPENDIX C

| Species | i | $l$ | $g_{il}$ | $\epsilon_{il}$ |
|---|---|---|---|---|
| $O^-$ | | 1 | 6 | 0 |
| C | | 1 | 9 | 0 |
| | | 2 | 5 | 10194 |
| | | 3 | 1 | 21648 |
| | | 4 | 5 | 33735 |
| | | 5 | 9 | 60360 |
| | | 6 | 3 | 61982 |
| | | 7 | 15 | 64090 |
| | | 8 | 3 | 68858 |
| | | 9 | 15 | 69700 |
| | | 10 | 3 | 70744 |
| | | 11 | 9 | 71365 |
| | | 12 | 5 | 72611 |
| | | 13 | 1 | 73976 |
| | | 14 | 9 | 75256 |
| | | 15 | 5 | 77681 |
| | | 16 | 9 | 78130 |
| | | 17 | 21 | 78230 |
| | | 18 | 18 | 78320 |
| | | 19 | 10 | 78600 |
| | | 20 | 9 | 79318 |
| | | 21 | 18 | 80400 |
| | | 22 | 12 | 81200 |
| | | 23 | 5 | 81770 |
| | | 24 | 1 | 82252 |
| | | 25 | 53 | 83800 |
| | | 26 | 103 | 84000 |
| | | 27 | 30 | 84940 |
| | | 28 | 6 | 85400 |
| | | 29 | 503 | 86400 |
| | | 30 | 19 | 86500 |

| Species | i | $l$ | $g_{il}$ | $\epsilon_{il}$ |
|---|---|---|---|---|
| $C^+$ | | 1 | 6 | 0 |
| | | 2 | 12 | 43030 |
| | | 3 | 10 | 74931 |
| | | 4 | 2 | 96494 |
| | | 5 | 6 | 101800 |
| | | 6 | 6 | 110650 |
| | | 7 | 2 | 114900 |
| | | 8 | 2 | 116538 |
| | | 9 | 14 | 119400 |
| | | 10 | 6 | 131731 |
| | | 11 | 12 | 135800 |
| | | 12 | 20 | 136000 |
| | | 13 | 4 | 142024 |
| | | 14 | 10 | 145551 |
| | | 15 | 10 | 150465 |
| | | 16 | 2 | 157234 |
| | | 17 | 6 | 162522 |
| | | 18 | 12 | 167000 |
| | | 19 | 10 | 168124 |
| | | 20 | 20 | 168900 |
| | | 21 | 2 | 173348 |
| | | 22 | 6 | 175293 |
| | | 23 | 16 | 178350 |
| | | 24 | 32 | 179000 |
| | | 25 | 26 | 182000 |
| | | 26 | 4 | 184689 |
| | | 27 | 12 | 186450 |
| | | 28 | 10 | 188600 |
| | | 29 | 30 | 195500 |
| | | 30 | 20 | 196572 |

| Species | i | $l$ | $g_{il}$ | $\epsilon_{il}$ |
|---|---|---|---|---|
| $C^{++}$ | | 1 | 1 | 0 |
| | | 2 | 9 | 52360 |
| | | 3 | 3 | 102351 |
| | | 4 | 9 | 137420 |
| | | 5 | 5 | 145875 |
| | | 6 | 1 | 182520 |
| | | 7 | 3 | 238161 |
| | | 8 | 1 | 247170 |
| | | 9 | 3 | 258931 |
| | | 10 | 9 | 259662 |
| | | 11 | 15 | 269960 |
| | | 12 | 5 | 276843 |
| | | 13 | 15 | 309100 |
| | | 14 | 1 | 311721 |
| | | 15 | 12 | 318700 |
| | | 16 | 61 | 322550 |
| | | 17 | 5 | 324212 |
| | | 18 | 12 | 328000 |
| | | 19 | 31 | 333000 |
| | | 20 | 15 | 337626 |
| | | 21 | 13 | 340000 |
| | | 22 | 7 | 341368 |
| | | 23 | 3 | 343256 |
| | | 24 | 30 | 345000 |
| | | 25 | 60 | 346600 |
| | | 26 | 7 | 348000 |
| | | 27 | 12 | 376600 |
| | | 28 | 18 | 381500 |
| | | 29 | 13 | 384345 |
| | | 30 | 34 | 386000 |

APPENDIX C

| Species | i | $l$ | $g_{il}$ | $\epsilon_{il}$ |
|---|---|---|---|---|
| $C^-$ | | 1 | 6 | 0 |
| A | | 1 | 1 | 0 |
| | | 2 | 5 | 93144 |
| | | 3 | 3 | 93751 |
| | | 4 | 1 | 94554 |
| | | 5 | 3 | 95400 |
| | | 6 | 3 | 104102 |
| | | 7 | 12 | 105500 |
| | | 8 | 8 | 106150 |
| | | 9 | 1 | 107054 |
| | | 10 | 8 | 107220 |
| | | 11 | 4 | 108000 |
| | | 12 | 4 | 111280 |
| | | 13 | 16 | 111750 |
| | | 14 | 8 | 112900 |
| | | 15 | 20 | 113550 |
| | | 16 | 16 | 114750 |
| | | 17 | 8 | 115000 |
| | | 18 | 3 | 116660 |
| | | 19 | 12 | 116960 |
| | | 20 | 8 | 117170 |
| | | 21 | 1 | 117563 |
| | | 22 | 16 | 118530 |
| | | 23 | 36 | 119300 |
| | | 24 | 56 | 120250 |
| | | 25 | 20 | 120700 |
| | | 26 | 32 | 121750 |
| | | 27 | 36 | 122200 |
| | | 28 | 56 | 122700 |
| | | 29 | 20 | 123500 |
| | | 30 | 28 | 124136 |

| Species | i | $l$ | $g_{il}$ | $\epsilon_{il}$ |
|---|---|---|---|---|
| $A^+$ | | 1 | 6 | 0 |
| | | 2 | 2 | 108723 |
| | | 3 | 20 | 132400 |
| | | 4 | 12 | 134800 |
| | | 5 | 6 | 138600 |
| | | 6 | 28 | 142700 |
| | | 7 | 6 | 145200 |
| | | 8 | 12 | 147650 |
| | | 9 | 10 | 148750 |
| | | 10 | 10 | 150000 |
| | | 11 | 12 | 155160 |
| | | 12 | 30 | 158300 |
| | | 13 | 12 | 161000 |
| | | 14 | 2 | 167309 |
| | | 15 | 14 | 170600 |
| | | 16 | 26 | 173000 |
| | | 17 | 38 | 174800 |
| | | 18 | 6 | 179700 |
| | | 19 | 40 | 183000 |
| | | 20 | 60 | 186000 |
| | | 21 | 62 | 190200 |
| | | 22 | 34 | 192200 |
| | | 23 | 120 | 194000 |
| | | 24 | 84 | 196000 |
| | | 25 | 48 | 200000 |
| | | 26 | 18 | 205000 |
| | | 27 | 6 | 208593 |
| | | 28 | 220 | 210000 |
| | | 29 | 50 | 215000 |
| | | 30 | 70 | 220000 |

| Species | i | $l$ | $g_{il}$ | $\epsilon_{il}$ |
|---|---|---|---|---|
| $A^{++}$ | | 1 | 5 | 0 |
| | | 2 | 3 | 1112 |
| | | 3 | 1 | 1570 |
| | | 4 | 5 | 14010 |
| | | 5 | 1 | 33267 |
| | | 6 | 9 | 114400 |
| | | 7 | 10 | 128000 |
| | | 8 | 28 | 144650 |
| | | 9 | 15 | 156950 |
| | | 10 | 5 | 174375 |
| | | 11 | 15 | 182000 |
| | | 12 | 75 | 189500 |
| | | 13 | 15 | 196600 |
| | | 14 | 5 | 200000 |
| | | 15 | 18 | 204700 |
| | | 16 | 21 | 208300 |
| | | 17 | 27 | 210800 |
| | | 18 | 33 | 214500 |
| | | 19 | 46 | 224500 |
| | | 20 | 9 | 231500 |
| | | 21 | 5 | 235000 |
| | | 22 | 26 | 240000 |
| | | 23 | 50 | 246036 |
| | | 24 | 91 | 251000 |
| | | 25 | 24 | 258000 |
| | | 26 | 127 | 270000 |
| | | 27 | 121 | 278500 |
| | | 28 | 116 | 282000 |
| | | 29 | 111 | 286000 |
| | | 30 | 524 | 302000 |

## APPENDIX C

| Species | $i$ | $l$ | $g_{il}$ | $\epsilon_{il}$ | $\Lambda_{il}$ | $\omega_{il1}$ | $\omega_{il2}$ | $\omega_{il3}$ | $\omega_{il4}$ |
|---|---|---|---|---|---|---|---|---|---|
| $N_2$ | | 1 | 1 | 0 | 5.725 | 2343.9 | 0 | 0 | 0 |
| | | 2 | 3 | 49757 | 4.125 | 1446.5 | 0 | 0 | 0 |
| | | 3 | 6 | 59314 | 4.687 | 1719.6 | 0 | 0 | 0 |
| | | 4 | 2 | 68953 | 4.630 | 1625.9 | 0 | 0 | 0 |
| | | 5 | 1 | 70700 | 4.235 | 1518.0 | 0 | 0 | 0 |
| | | 6 | 6 | 87984 | 5.226 | 2018.0 | 0 | 0 | 0 |
| $N_2^+$ | | 1 | 2 | 0 | 5.531 | 2191.0 | 0 | 0 | 0 |
| | | 2 | 4 | 9020 | 4.929 | 1887.9 | 0 | 0 | 0 |
| | | 3 | 2 | 25570 | 5.966 | 2396.7 | 0 | 0 | 0 |
| | | 4 | 2 | 64550 | 4.676 | 2035.1 | 0 | 0 | 0 |
| $O_2$ | | 1 | 3 | 0 | 4.137 | 1568.3 | 0 | 0 | 0 |
| | | 2 | 2 | 7882 | 4.080 | 1496.4 | 0 | 0 | 0 |
| | | 3 | 1 | 13121 | 4.004 | 1418.7 | 0 | 0 | 0 |
| | | 4 | 3 | 35713 | 2.970 | 796.5 | 0 | 0 | 0 |
| | | 5 | 1 | 36213 | 2.347 | 633.3 | 0 | 0 | 0 |
| | | 6 | 3 | 49363 | 2.341 | 692.4 | 0 | 0 | 0 |
| $O_2^+$ | | 1 | 4 | 0 | 4.783 | 1859.9 | 0 | 0 | 0 |
| | | 2 | 8 | 31500 | 3.156 | 1025.3 | 0 | 0 | 0 |
| | | 3 | 4 | 38300 | 3.028 | 886.6 | 0 | 0 | 0 |
| | | 4 | 4 | 48100 | 3.673 | 1179.7 | 0 | 0 | 0 |
| $O_2^-$ | | 1 | 4 | 0 | 3.430 | 1286.0 | 0 | 0 | 0 |
| | | 2 | 4 | 13400 | 2.767 | 975.0 | 0 | 0 | 0 |
| | | 3 | 4 | 24200 | 2.609 | 547.0 | 0 | 0 | 0 |
| NO | | 1 | 2 | 0 | 2.440 | 1890.1 | 0 | 0 | 0 |
| | | 2 | 2 | 121 | 2.440 | 1889.7 | 0 | 0 | 0 |
| | | 3 | 2 | 44200 | 2.860 | 2358.3 | 0 | 0 | 0 |
| | | 4 | 4 | 45440 | 1.609 | 1030.1 | 0 | 0 | 0 |
| | | 5 | 2 | 53290 | 2.866 | 2301.0 | 0 | 0 | 0 |
| | | 6 | 4 | 52376 | 2.859 | 2380.0 | 0 | 0 | 0 |
| | | 7 | 2 | 60860 | 2.845 | 2357.8 | 0 | 0 | 0 |
| | | 8 | 4 | 60020 | 1.900 | 1200.7 | 0 | 0 | 0 |
| $NO^+$ | | 1 | 1 | 0 | 2.866 | 2360.8 | 0 | 0 | 0 |
| | | 2 | 6 | 39982 | 2.404 | 1725.5 | 0 | 0 | 0 |
| | | 3 | 3 | 58523 | 1.902 | 1210.5 | 0 | 0 | 0 |
| | | 4 | 6 | 72384 | 1.801 | 1132.4 | 0 | 0 | 0 |
| | | 5 | 2 | 73084 | 2.266 | 1585.6 | 0 | 0 | 0 |
| CO | | 1 | 1 | 0 | 2.766 | 2156.8 | 0 | 0 | 0 |
| | | 2 | 6 | 48474 | 2.405 | 1724.8 | 0 | 0 | 0 |
| | | 3 | 3 | 55380 | 1.904 | 1208.5 | 0 | 0 | 0 |
| | | 4 | 6 | 61785 | 1.803 | 1130.2 | 0 | 0 | 0 |
| | | 5 | 2 | 64747 | 2.303 | 1498.4 | 0 | 0 | 0 |
| | | 6 | 3 | 83831 | 2.962 | 2184.5 | 0 | 0 | 0 |
| | | 7 | 1 | 86918 | 2.802 | 2070.0 | 0 | 0 | 0 |
| $CO^+$ | | 1 | 2 | 0 | 2.831 | 2199.1 | 0 | 0 | 0 |
| | | 2 | 4 | 20407 | 2.273 | 1548.5 | 0 | 0 | 0 |
| | | 3 | 2 | 45634 | 2.568 | 1706.3 | 0 | 0 | 0 |
| CN | | 1 | 2 | 0 | 2.7207 | 2055.56 | 0 | 0 | 0 |
| | | 2 | 4 | 9115 | 2.4571 | 1801.55 | 0 | 0 | 0 |
| | | 3 | 2 | 25798 | 2.8186 | 2143.88 | 0 | 0 | 0 |
| $CO_2$ | | 1 | 1 | 0 | 1.121 | 667.3 | 667.3 | 1342.9 | 2349.3 |
| $N_2O$ | | 1 | 1 | 0 | .6017 | 588.8 | 588.8 | 1285.0 | 2223.8 |

## REFERENCES


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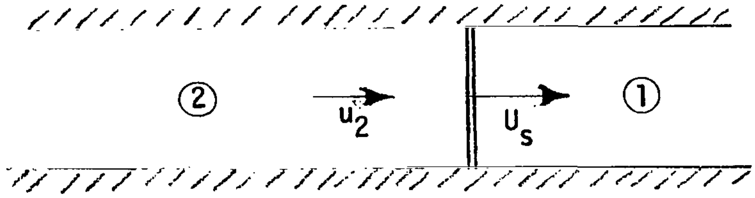
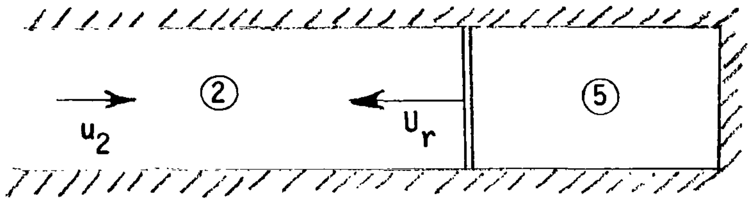
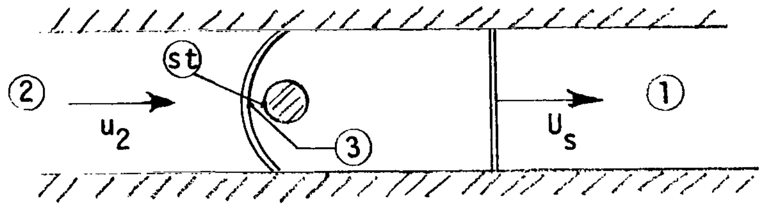


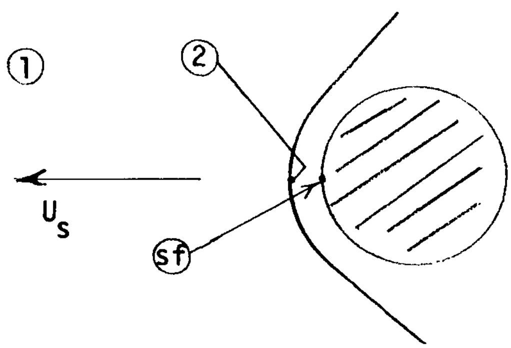

(a) Traveling normal shock.




(b) Reflected normal shock.

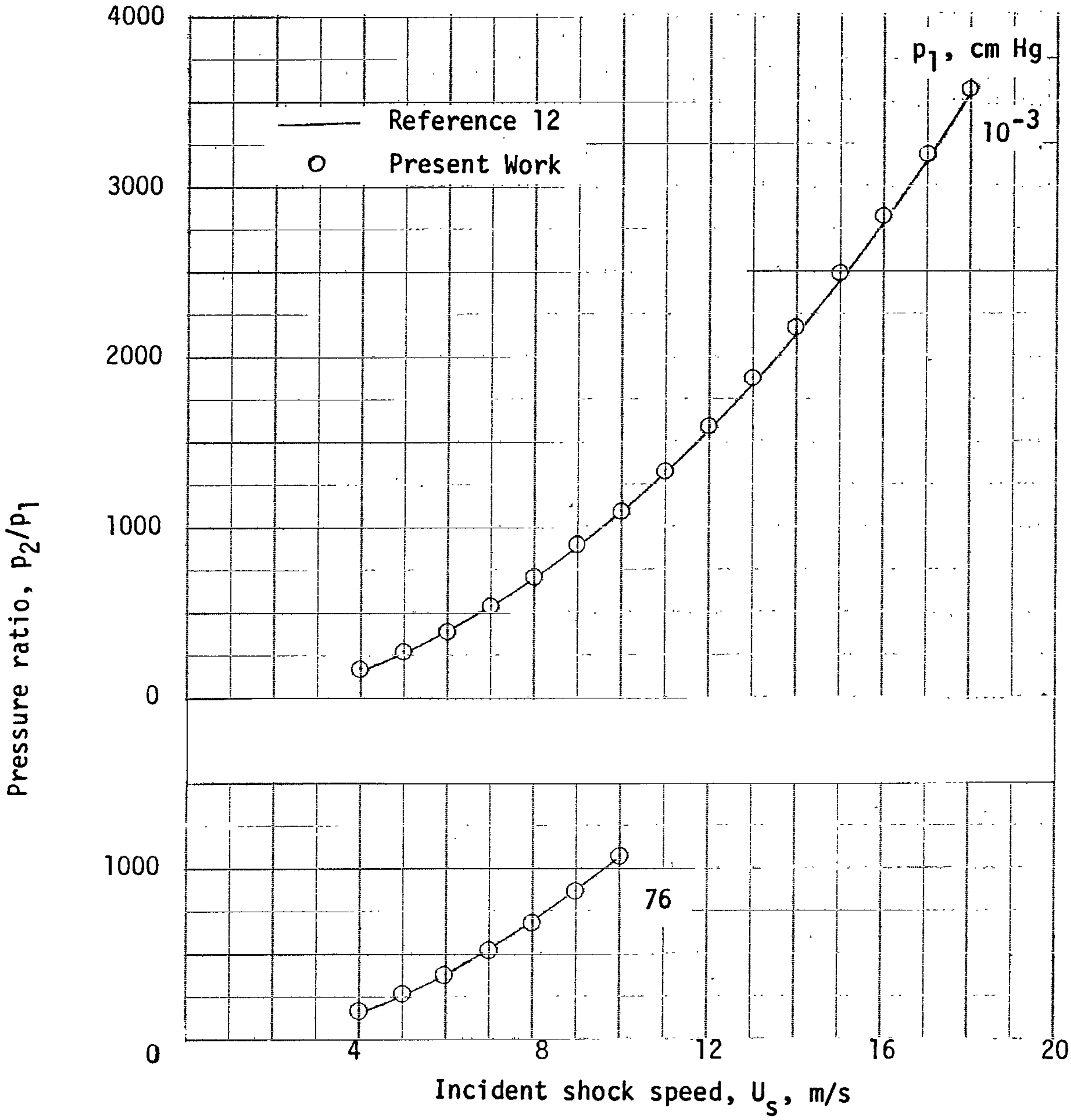



(c) Shock-tube stagnation point.



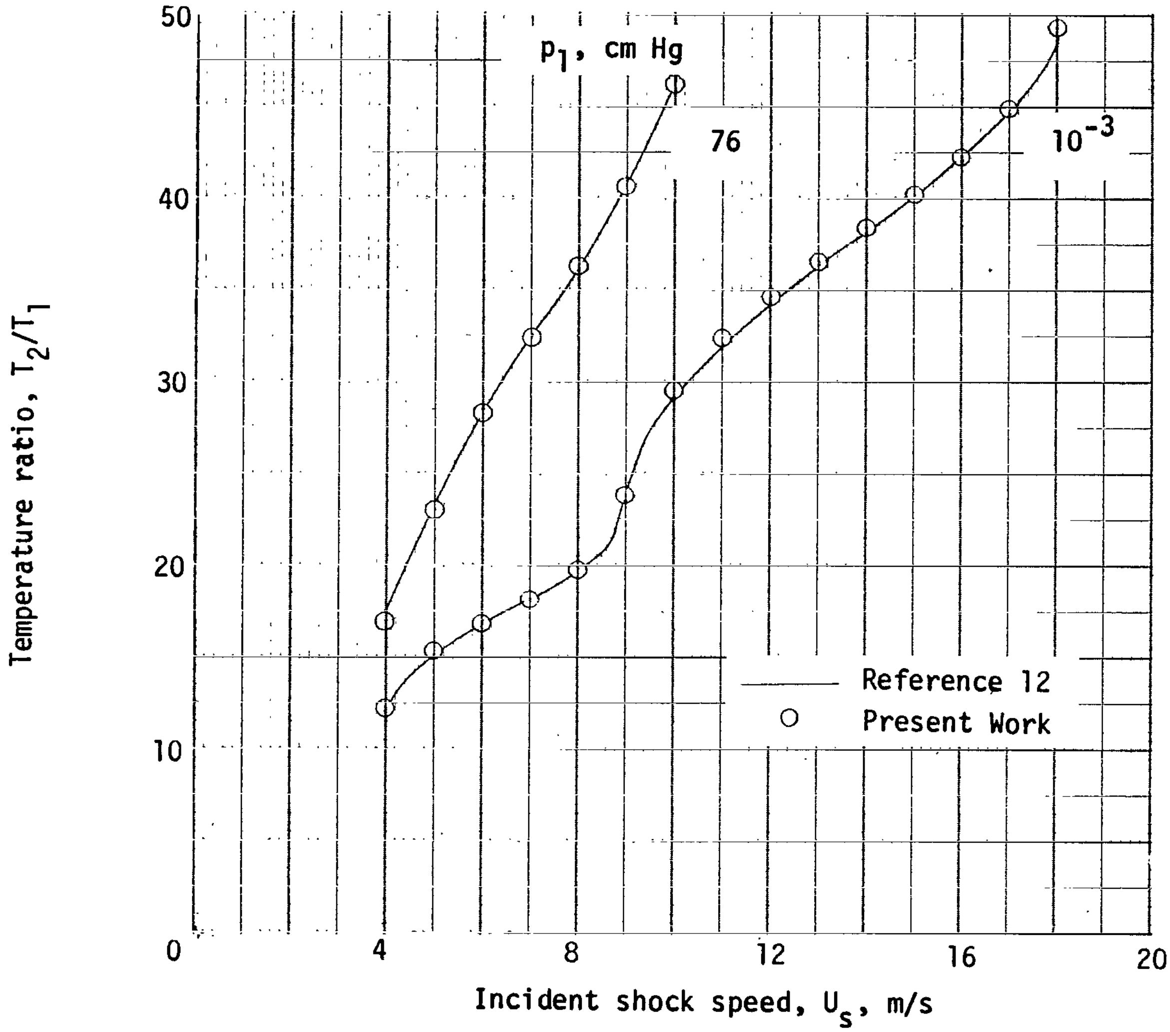

(d) In-flight stagnation point.

Figure 1.- Flow configurations.



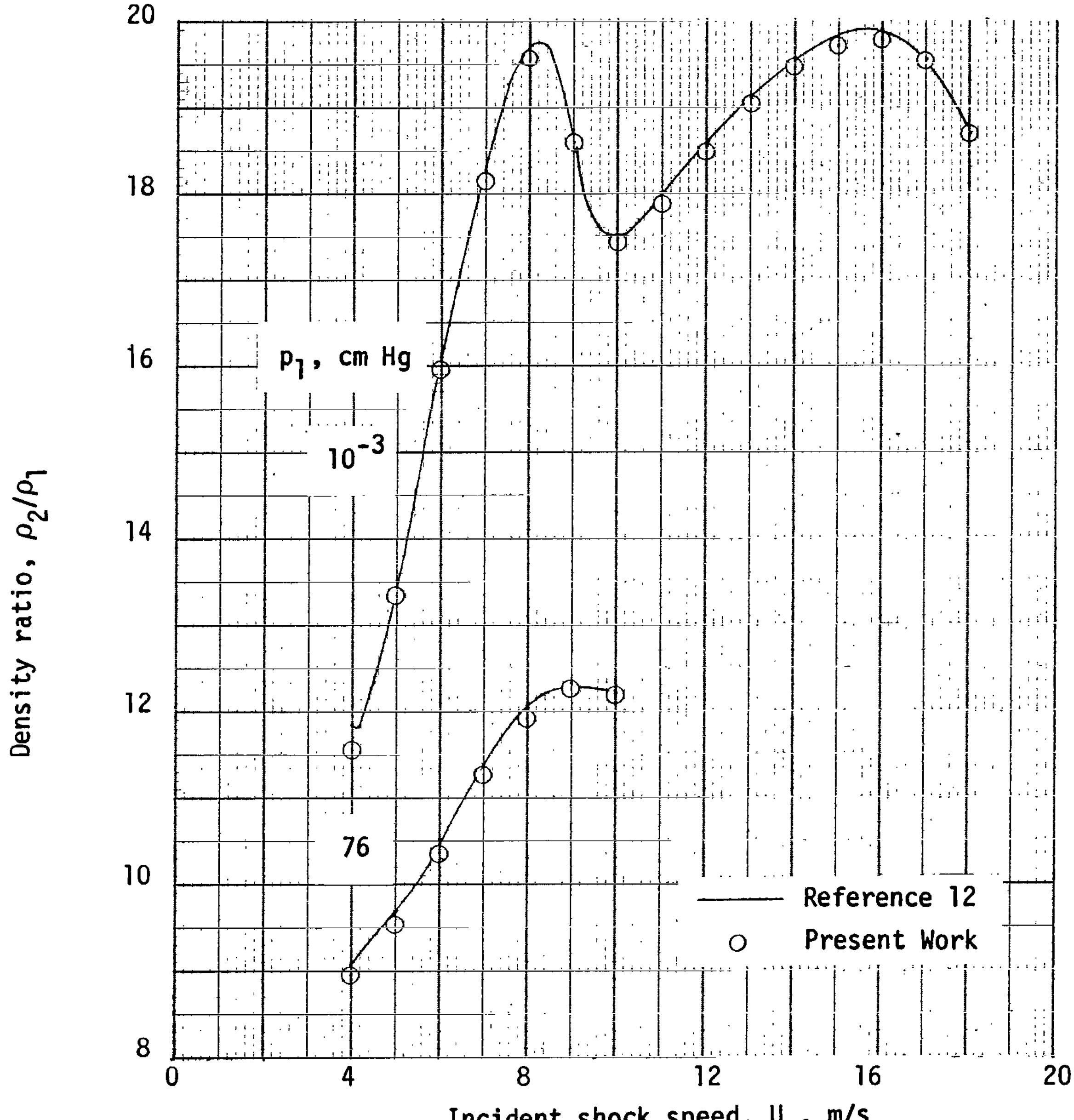

(a) Pressure.

Figure 2.- Thermodynamic ratios across traveling normal shock for carbon and argon free air. $T_1 = 300^{\circ}$ K.



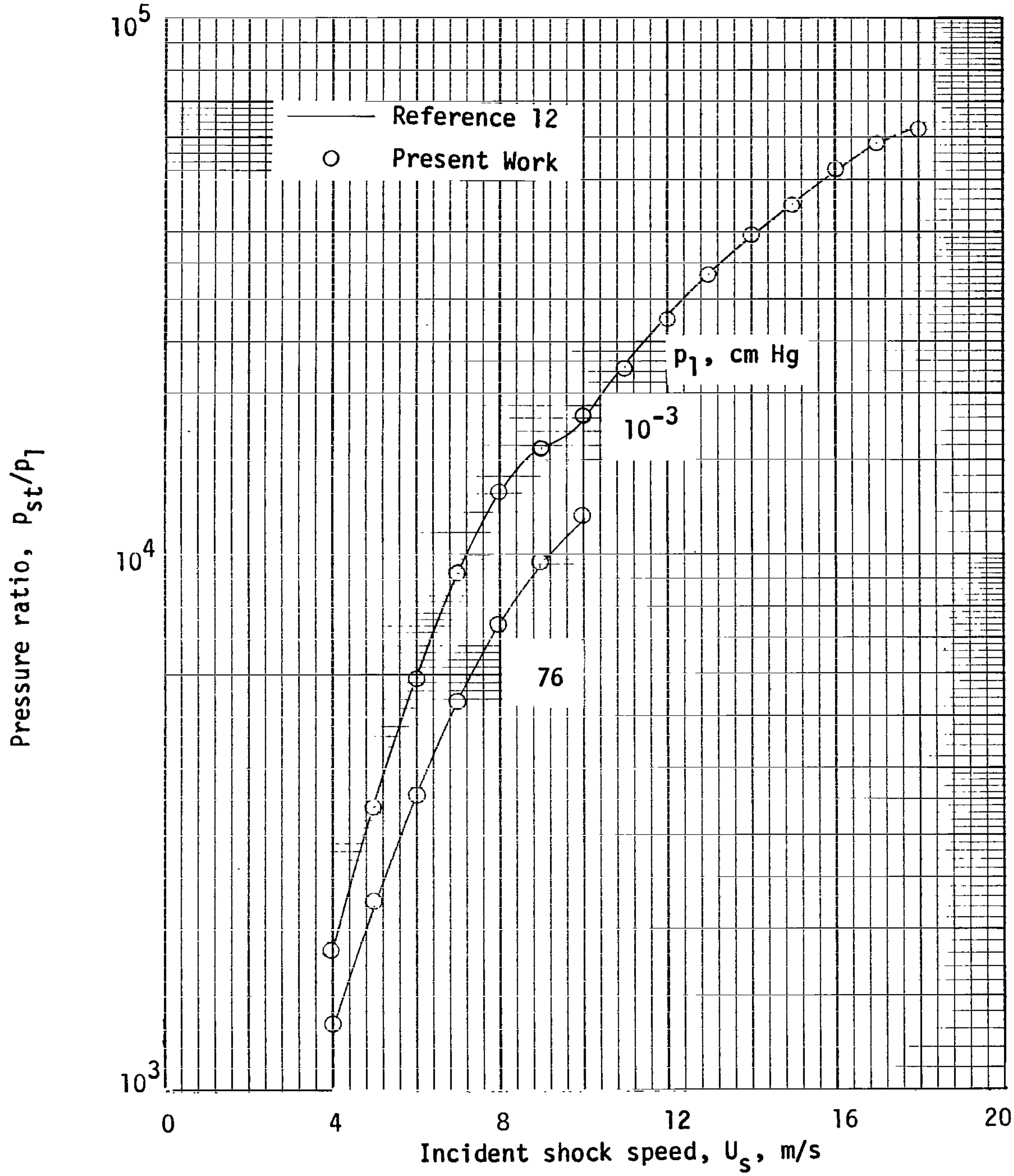

(b) Temperature.

Figure 2.- Continued.



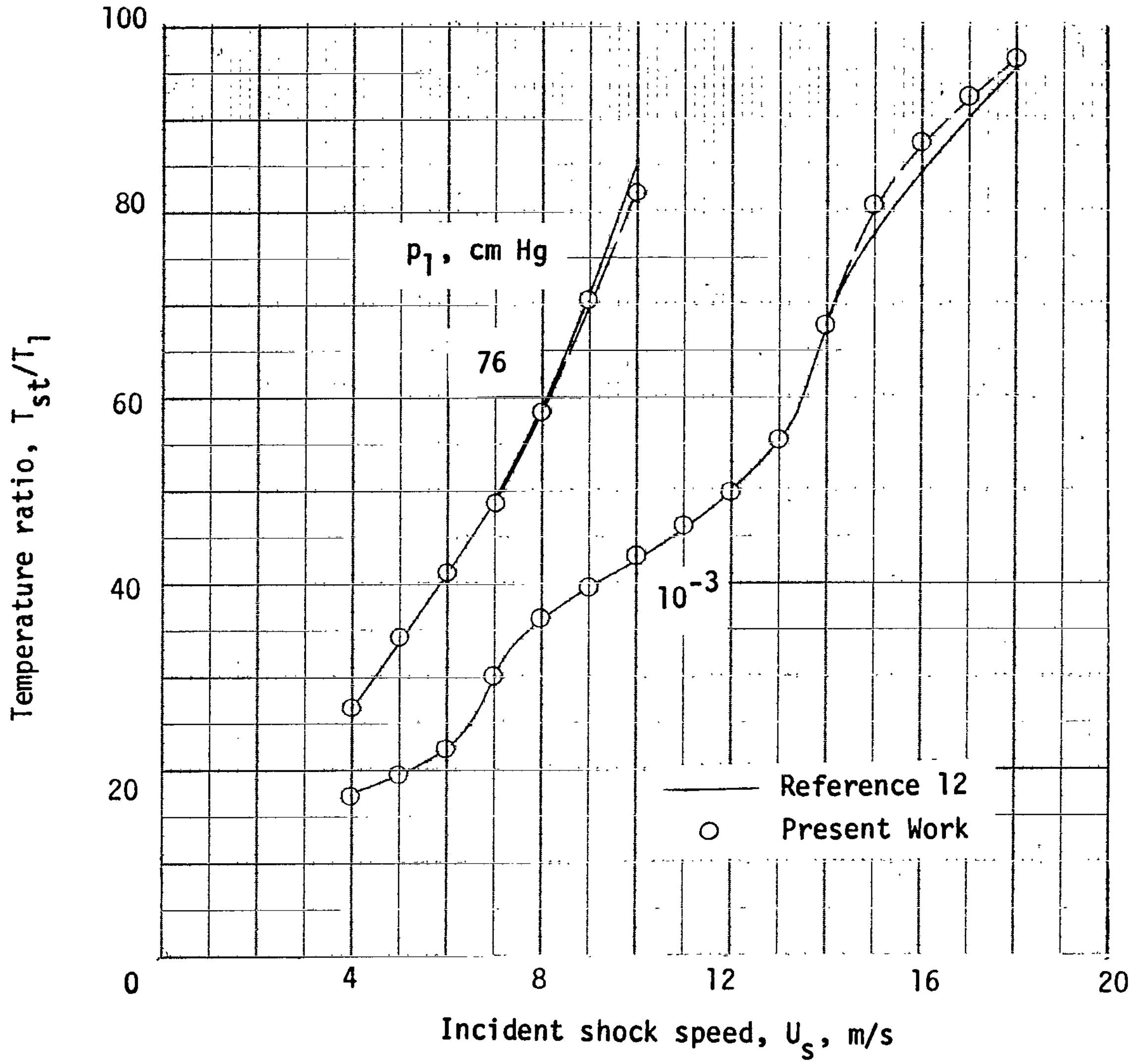

(c) Density.

Figure 2.- Concluded.



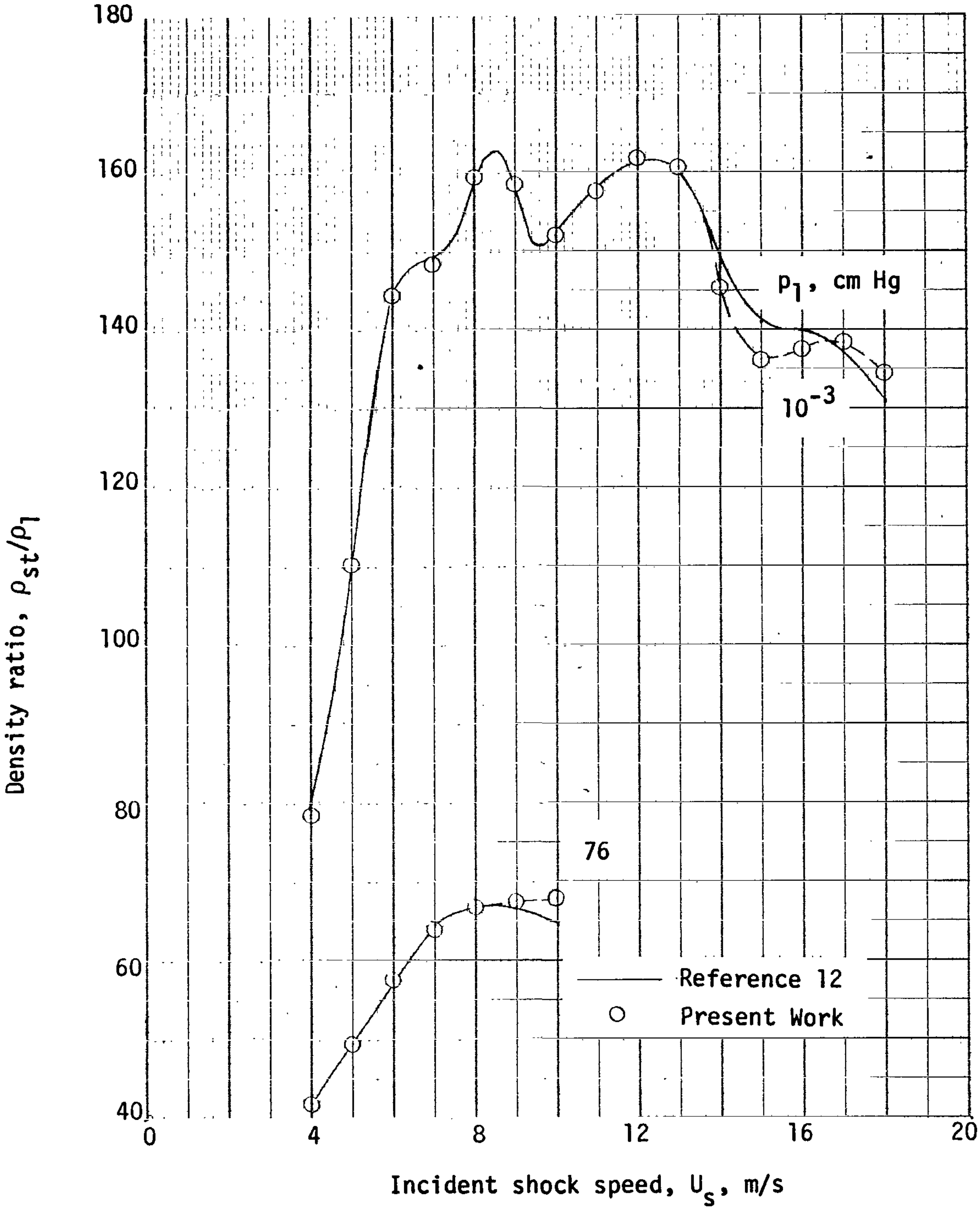

(a) Pressure.

Figure 3.- Shock-tube stagnation-point conditions for carbon and argon free air. $T_1 = 300^\circ$ K.




(b) Temperature.

Figure 3.- Continued.




(c) Density.

Figure 3.- Concluded.

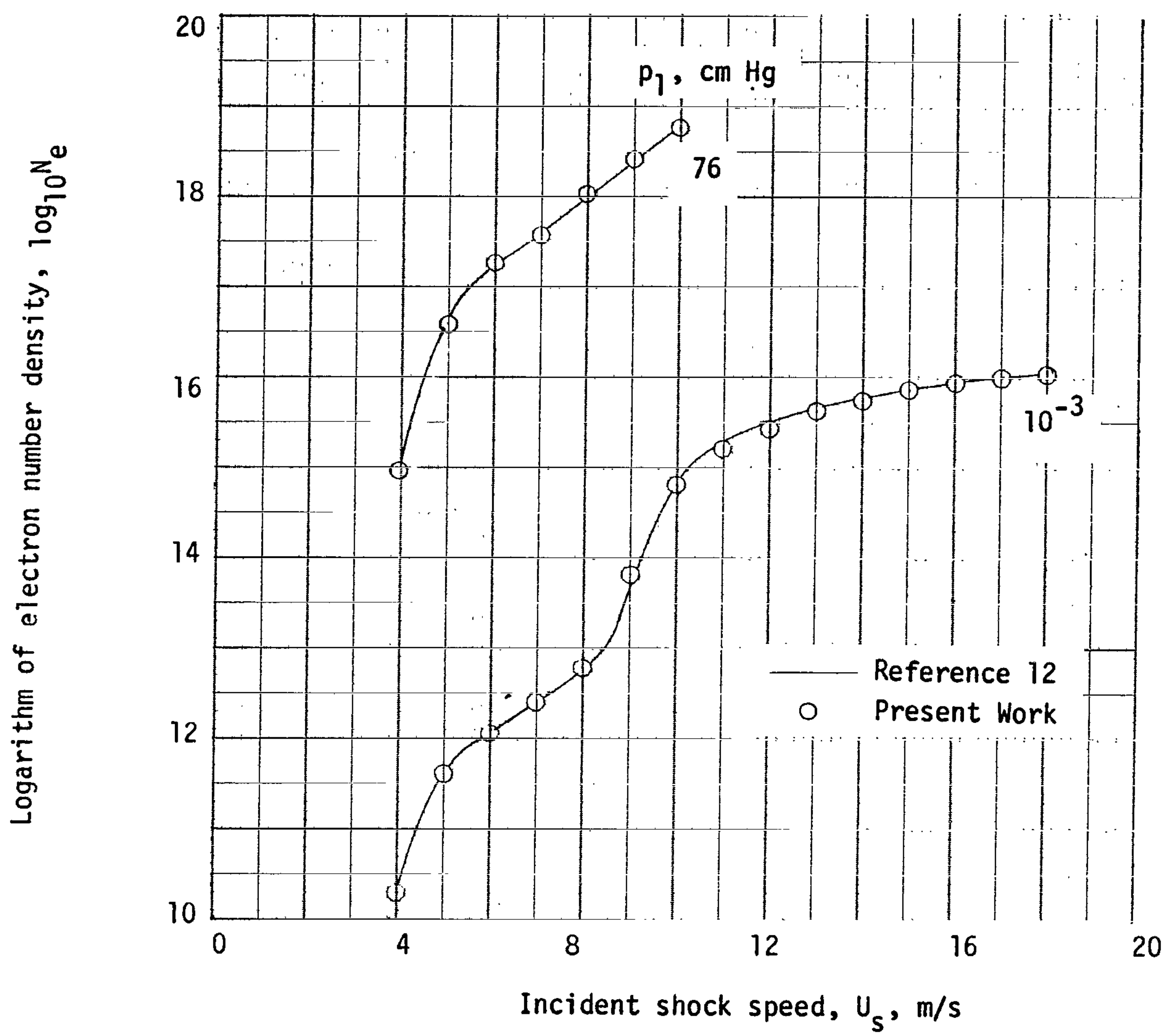



Figure 4.- Electron number density behind incident shock in particles per cubic centimeter for carbon and argon free air. $T_1 = 300^{\circ}$ K.

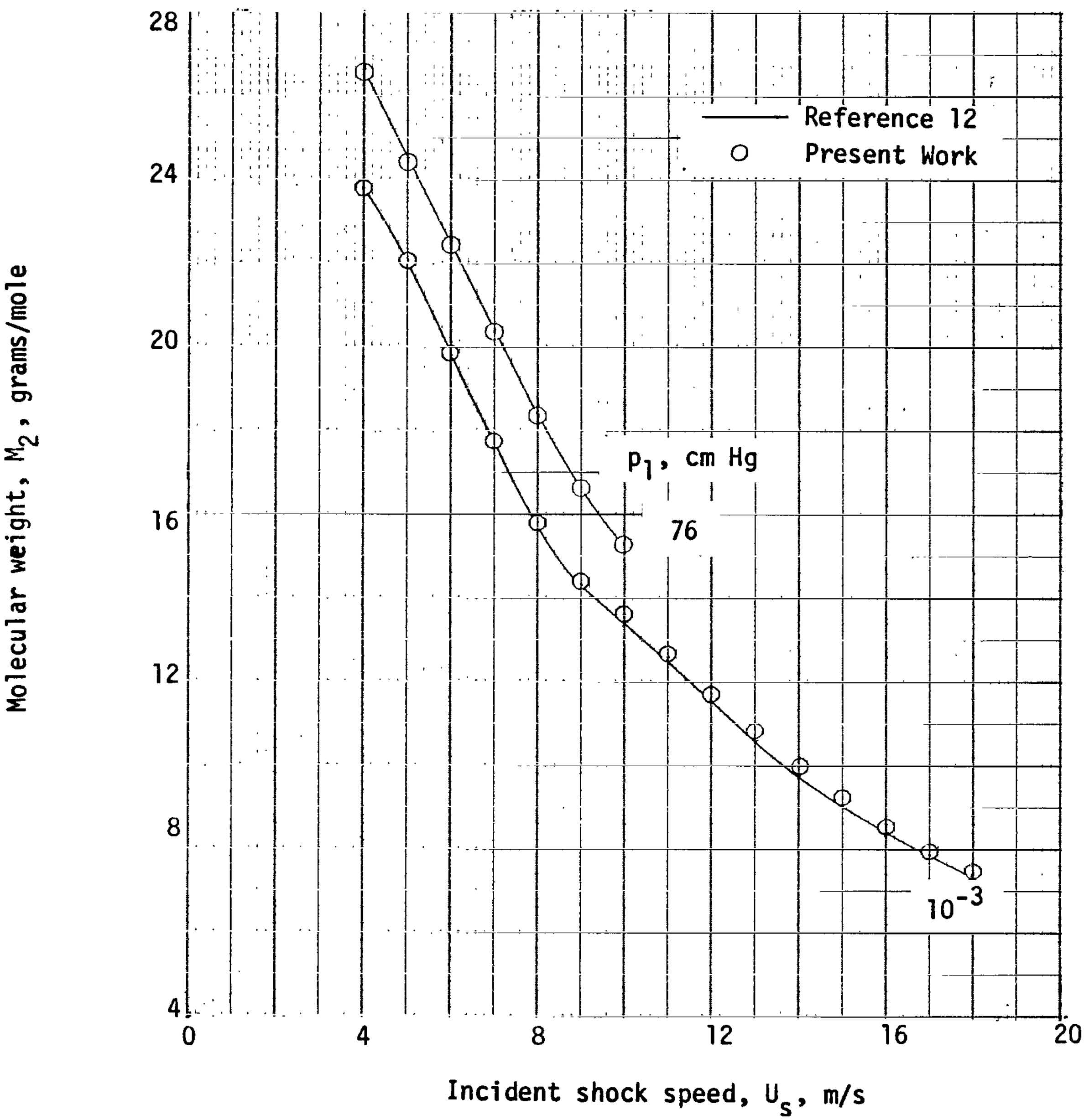
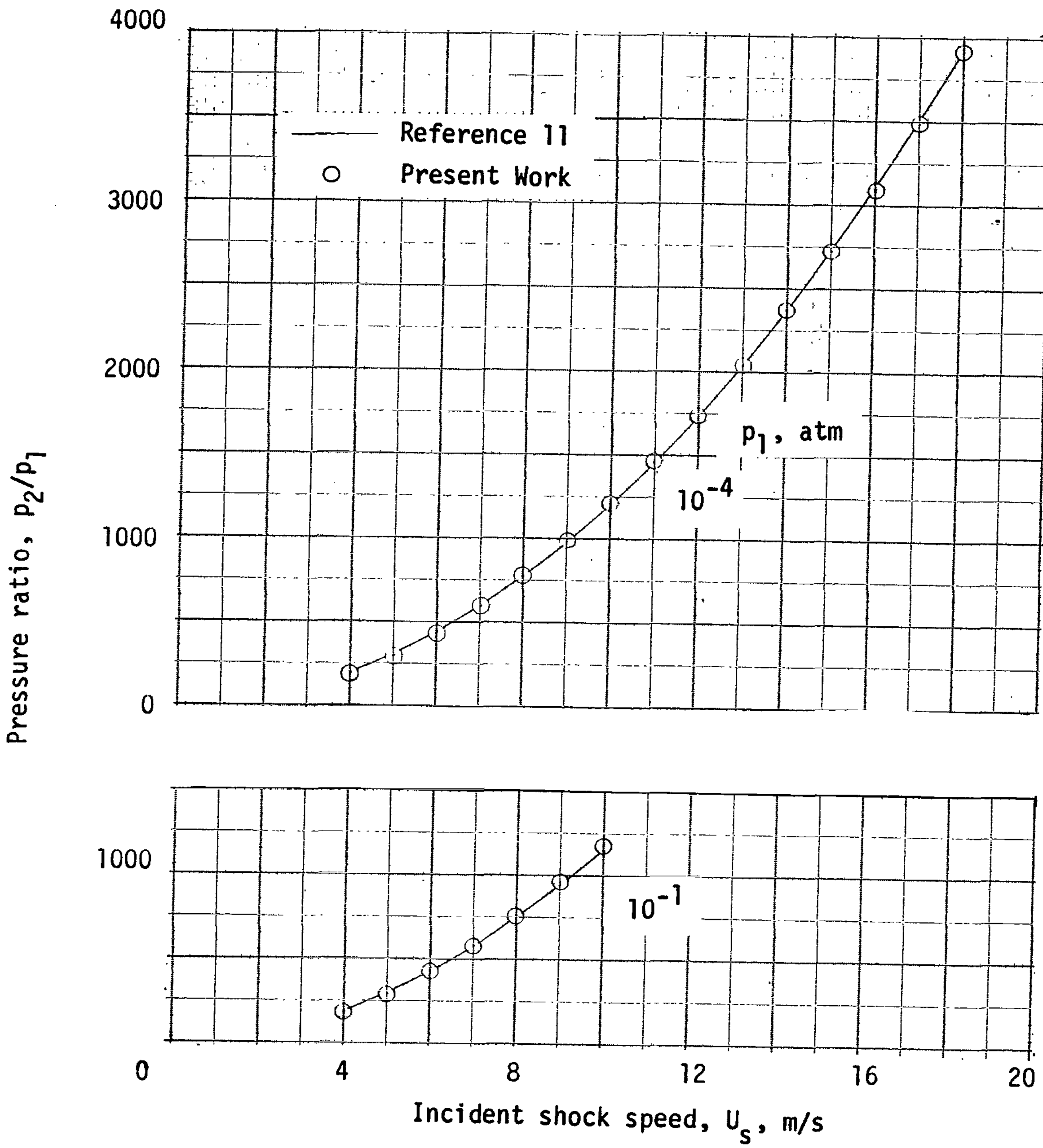
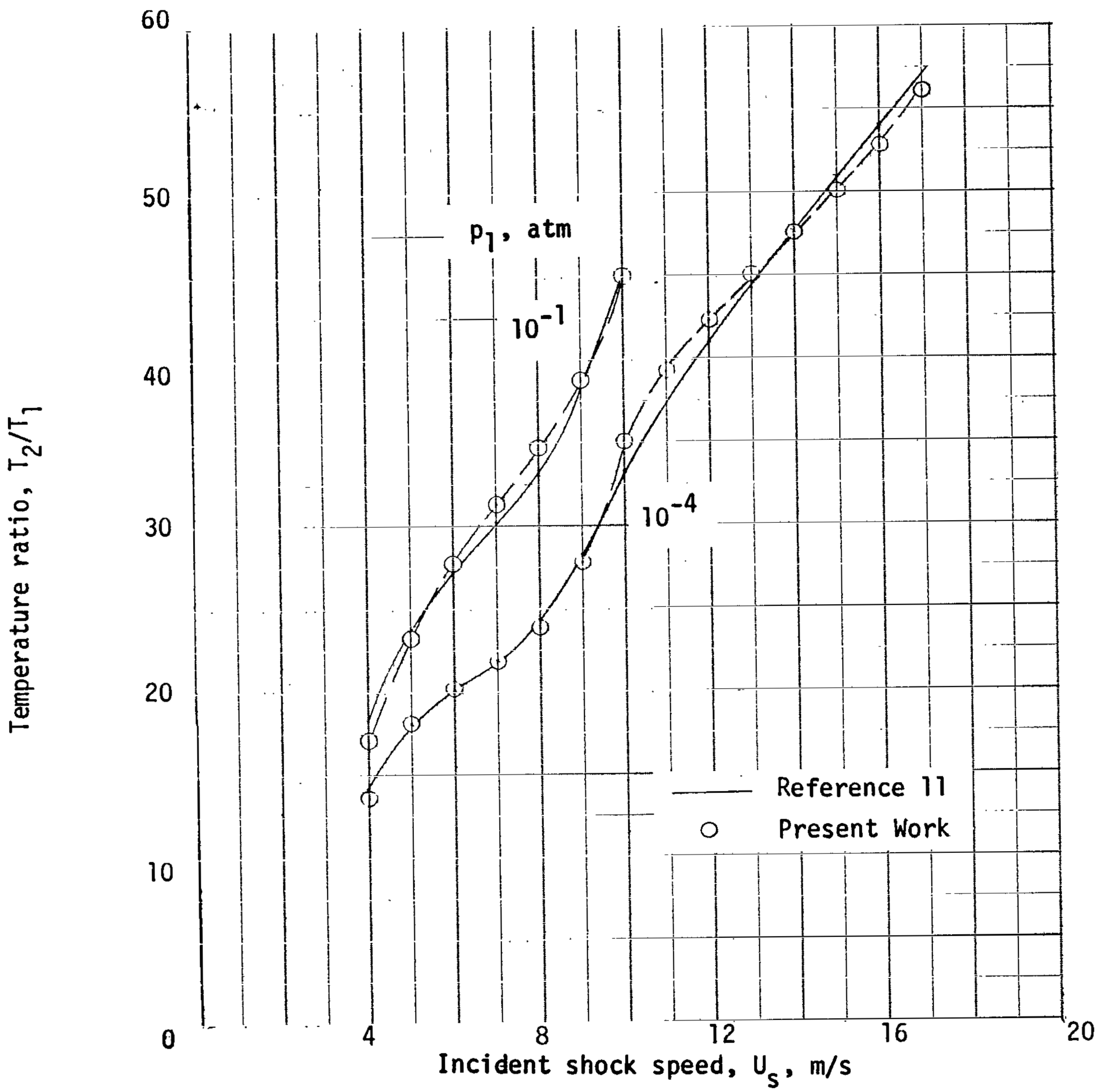



Figure 5.- Molecular weight behind incident shock for carbon and argon free air. $T_1 = 300^\circ$ K.



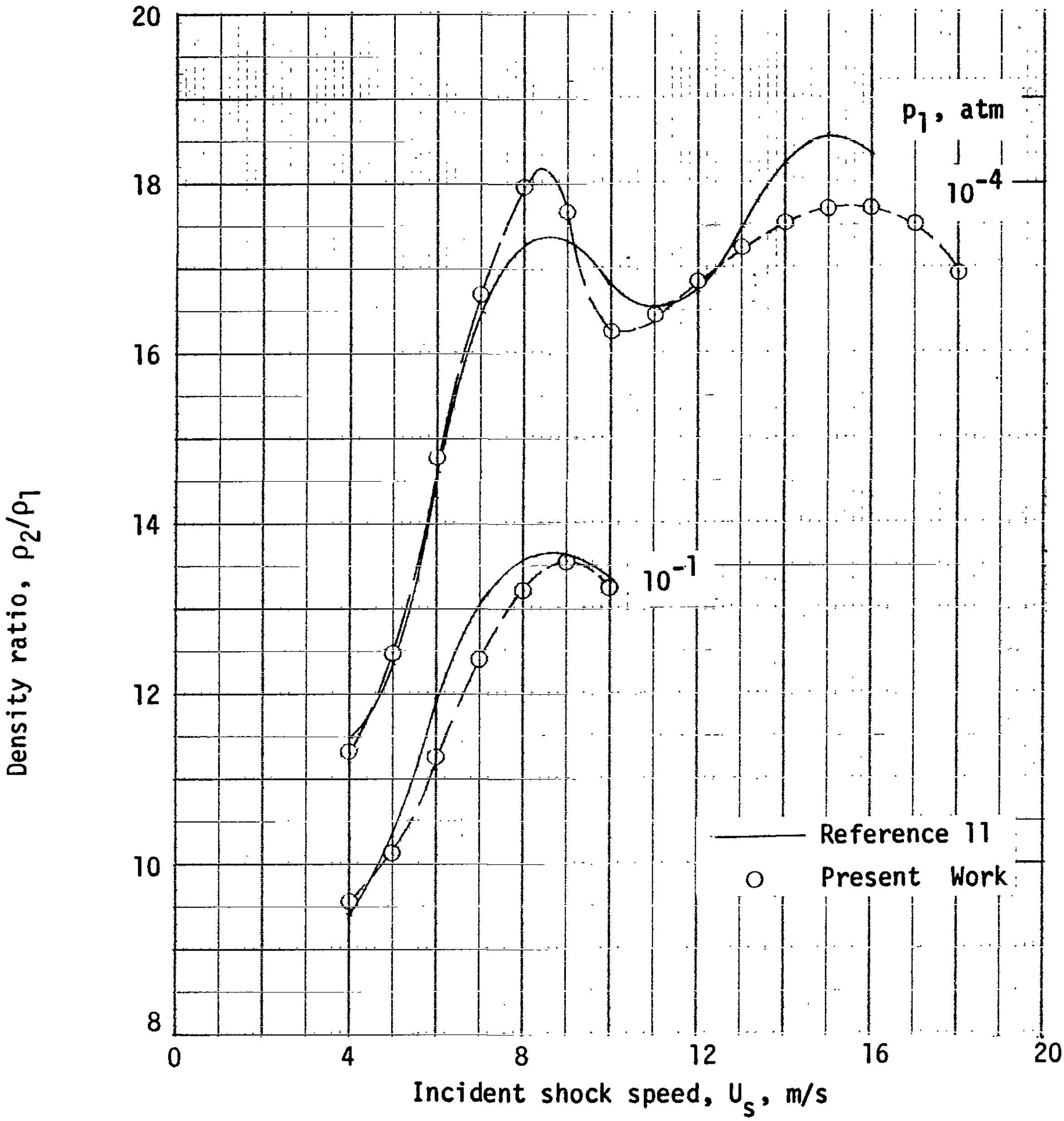

(a) Pressure.

Figure 6.- Thermodynamic ratios across traveling normal shock for carbon and argon free air. $T_1 = 273.2^\circ$ K.



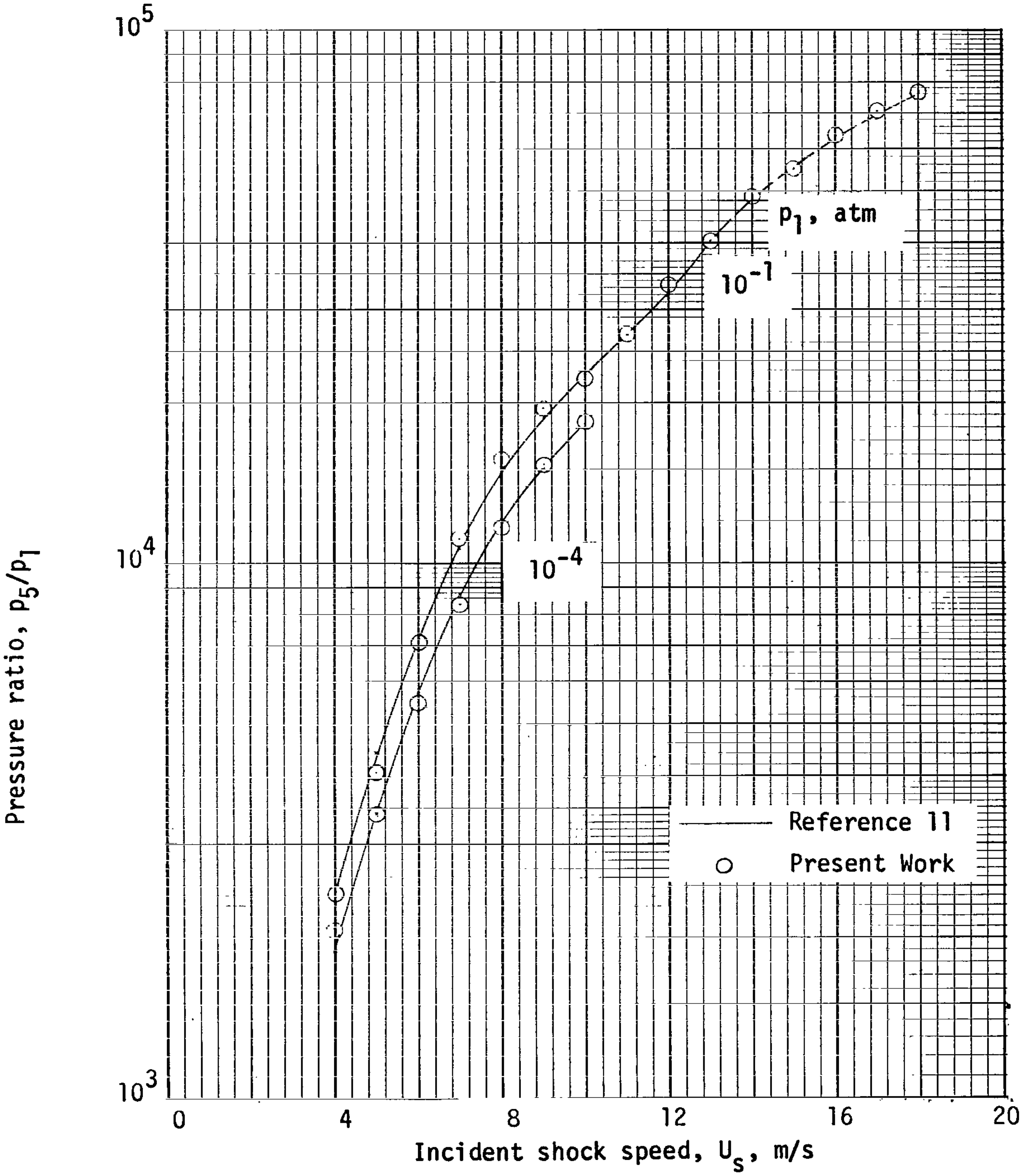

(b) Temperature.

Figure 6.- Continued.



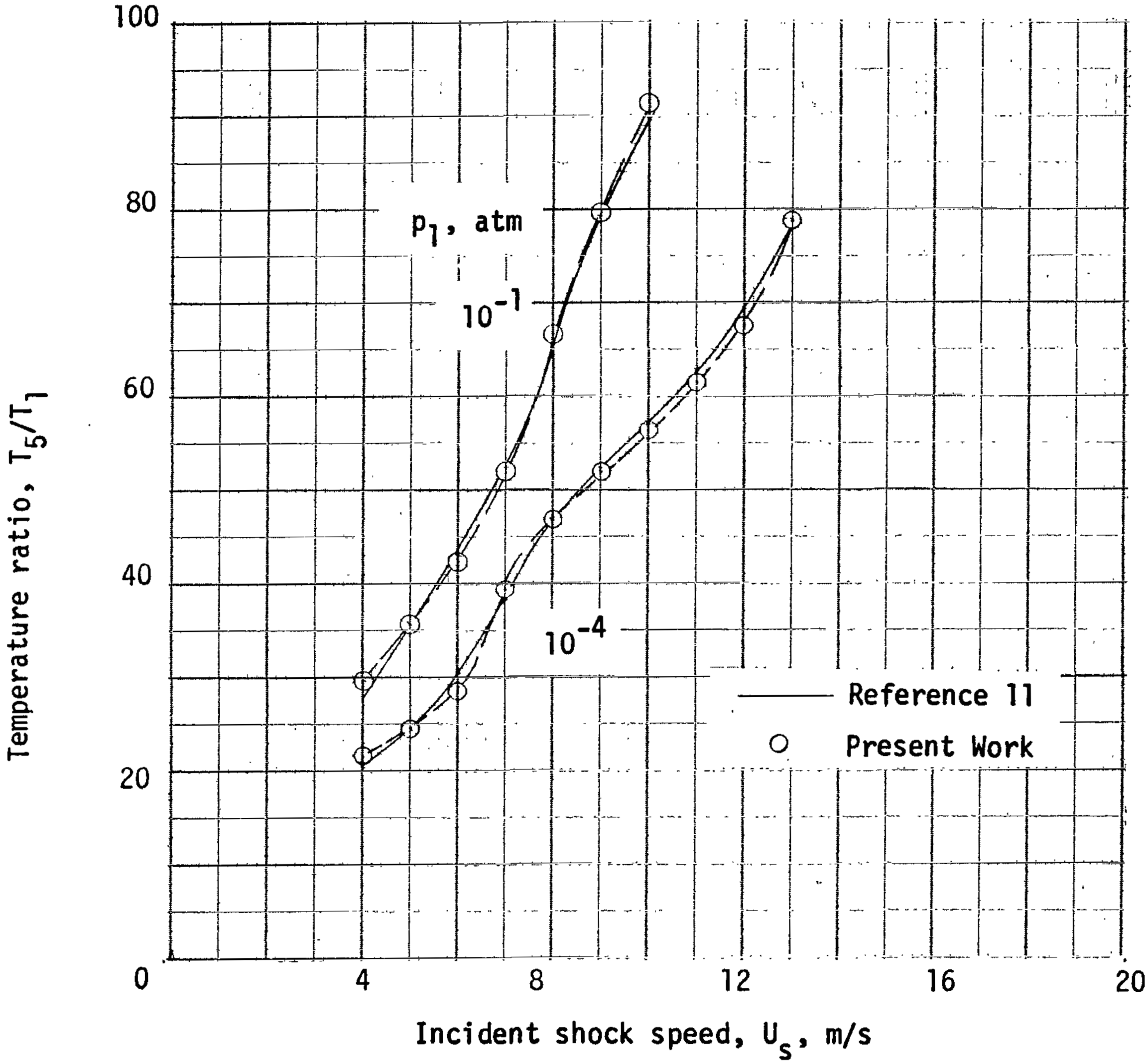

(c) Density.

Figure 6.- Concluded.



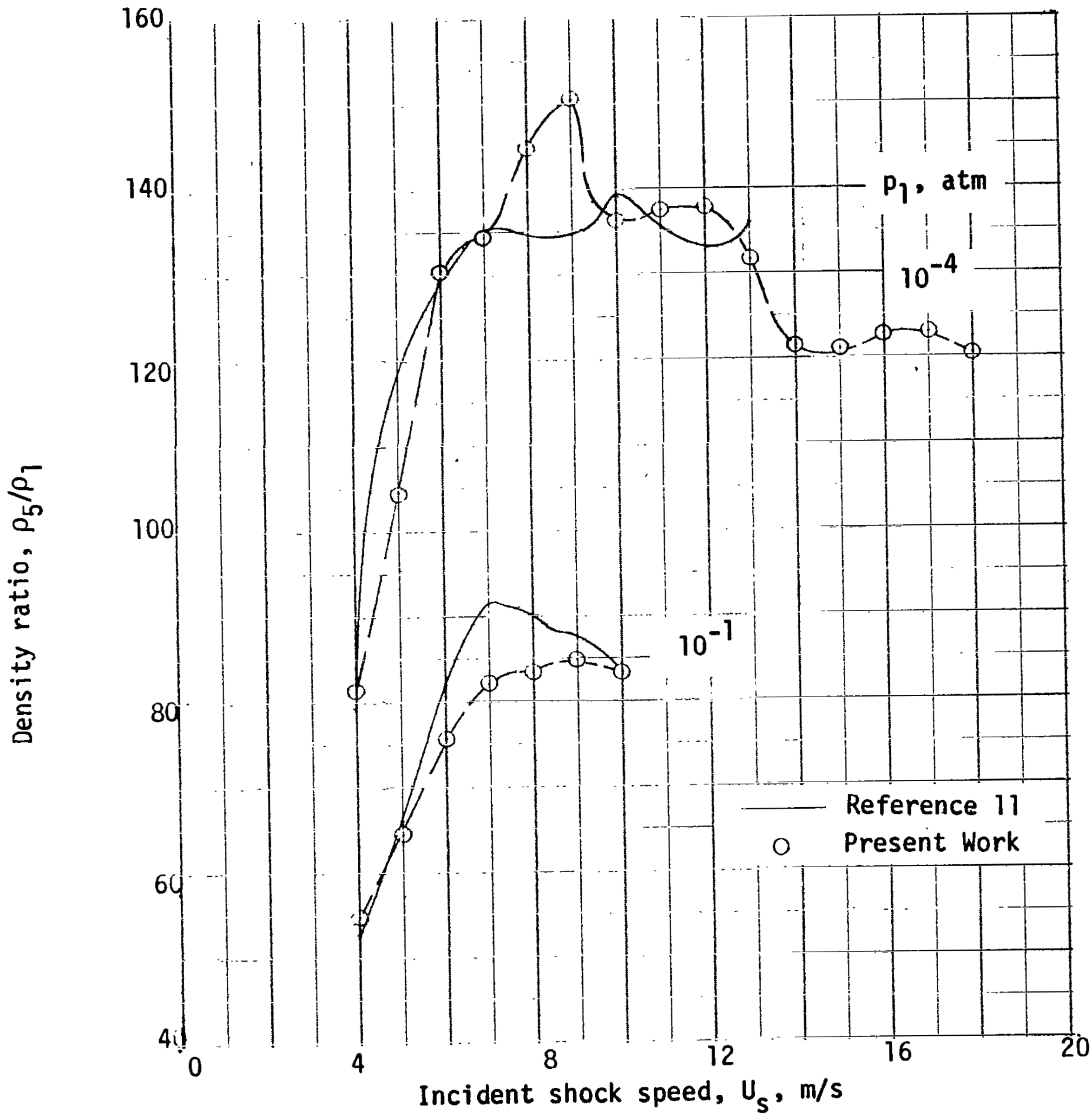

(a) Pressure.

Figure 7.- Thermodynamic ratios across reflected normal shock for carbon and argon free air. $T_1 = 273.2^{\circ}$ K.



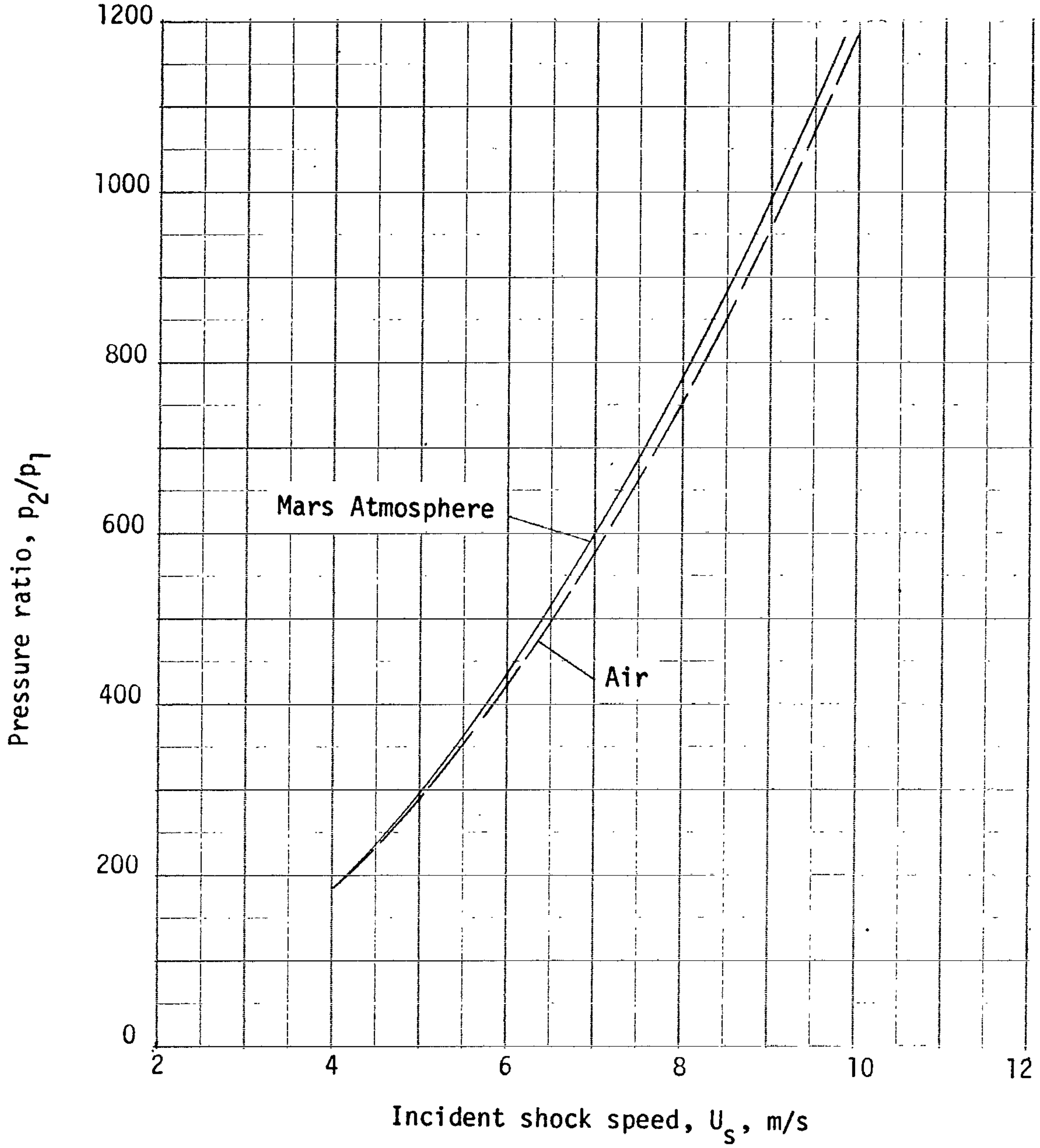

(b) Temperature.

Figure 7.- Continued.



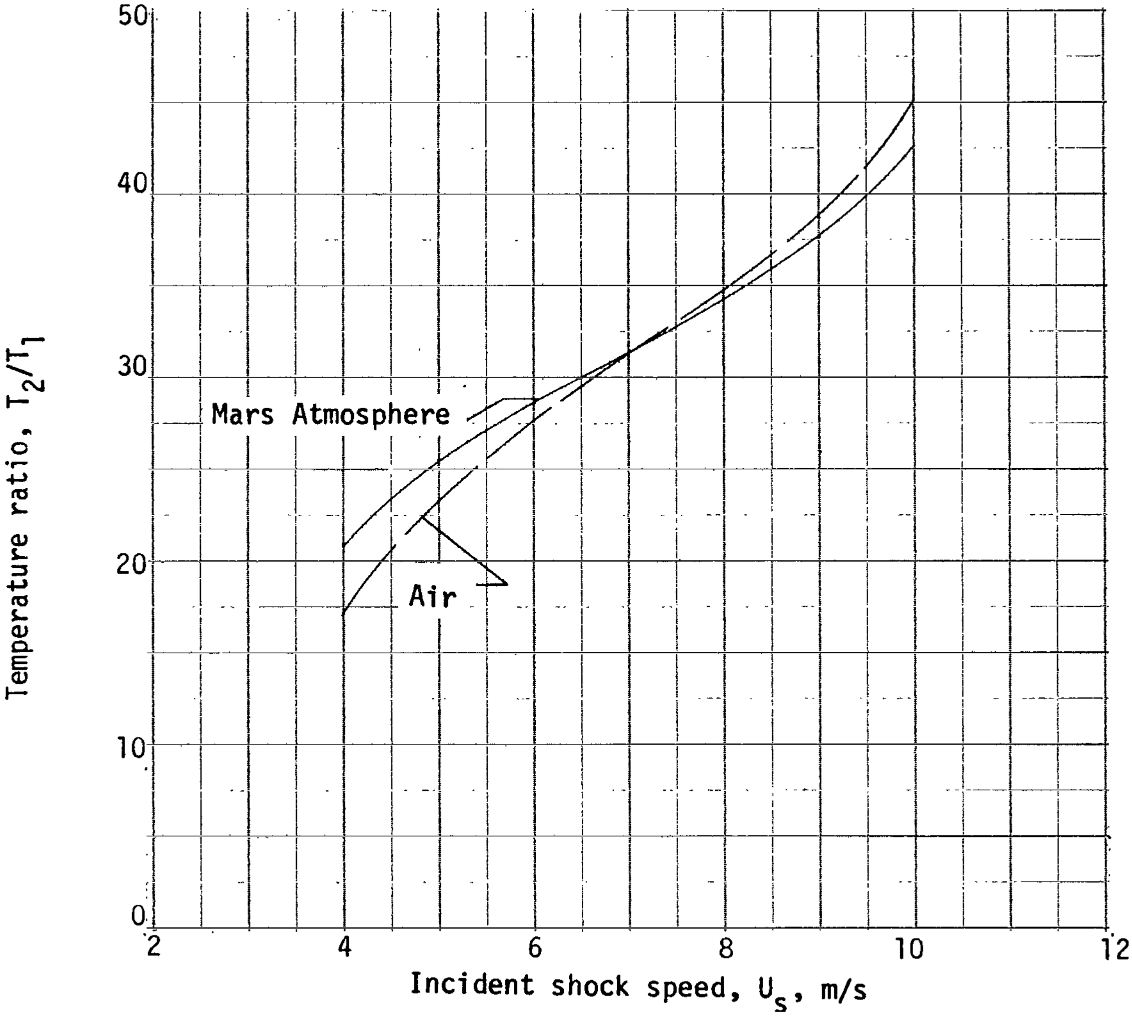

(c) Density.

Figure 7.- Concluded.



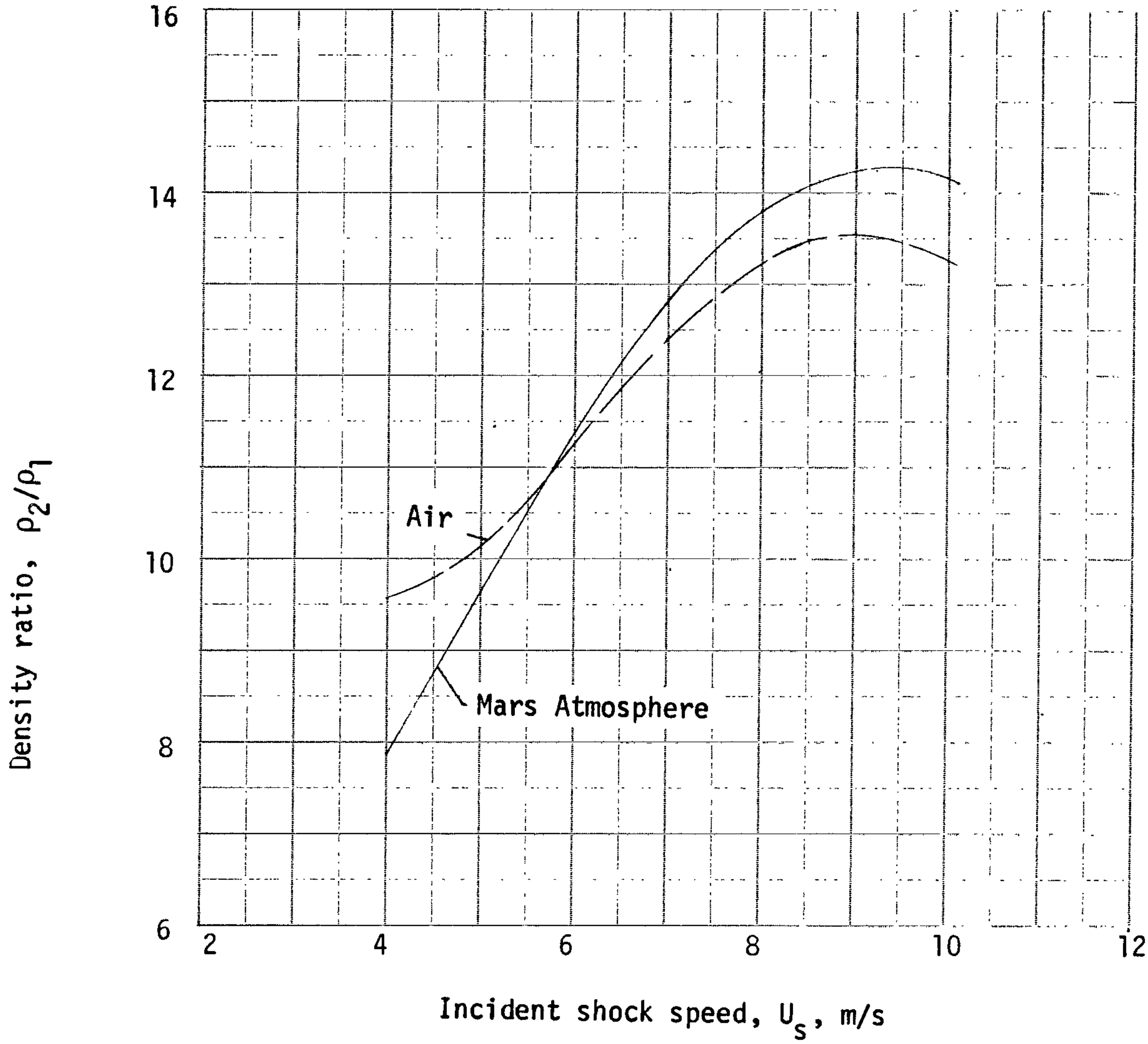

(a) Pressure.

Figure 8.- Comparison of normal shock properties for Martian atmosphere (NASA model 2, ref. 14) and for air. $T_1 = 273.2^\circ$ K; $p_1 = 10^{-1}$ atm.




(b) Temperature.

Figure 8.- Continued.




(c) Density.

Figure 8.- Concluded.



NASA-Langley, 1966 L-4399

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